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www.vishwabharati.in ISSN 2320-6263

RESEARCH ARENA

A MULTI-DISCIPLINARY INTERNATIONAL REFEREED RESEARCH JOURNAL

Vol 9 ● Issue 3 ● June 2021

RESEARCH ARENA
ISSN 2320-6263
Vol 10. Issue 3. June 2021. pp. 7-11
Paper received: 04 May 2021.
Paper accepted: 11 May 2021.

Enhancing MNCs' Contribution to Indian Economy

Devendrappa S. Nittur

Introduction:

Multinational corporations, as the name implies, are large corporate institutions. They have a variety of business interests. With their headquarters in one country, they carry on their business in more than one country. There are a number of criteria to define a multinational company. But the only criterion that comes to mind is their global and transnational activities. A multinational corporation can also be referred to as a multinational enterprise (MNE), a transnational enterprise (TNE), a transnational corporation (TNC), an international corporation, or a stateless corporation. There are subtle but real differences between these terms.

Globalization since its advent has been looked at suspiciously as a means of the developed nations bringing the developing nations in line with their own interests. Globalization and economic liberalization came as a pioneer of new hopes and developing nations were promised economic prosperity. In isolation, they could not survive, they were told. The World Trade Organisation

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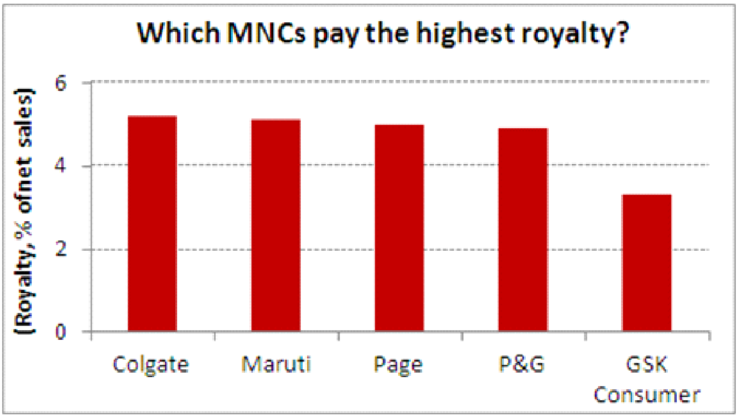
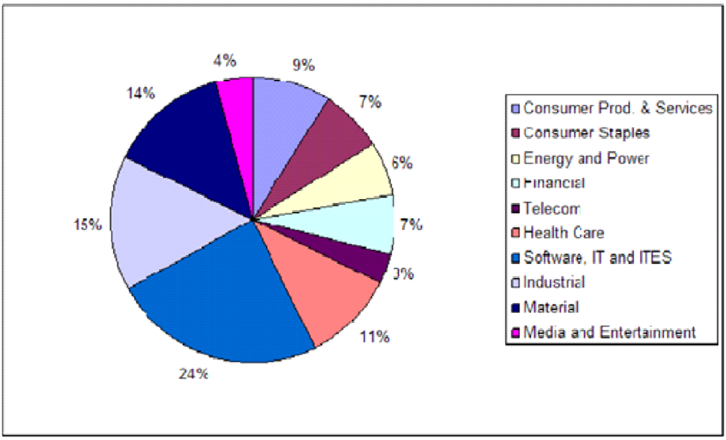
(WTO) is the organization which ensures that globalization works in favour of developed countries. Various WTO ministerial conferences show that globalization has not proved what it promised to be. MNCs from the economically developed countries establish their outlets in the areas that benefit them. They would not invest in the sectors beneficial for the developing countries. Even in India, production is guided by MNCs. In international conferences the developed nations defend the interests of their own MNCs with authority.

What is the real truth about the multinational operations in the context of India? Multinationals are not an unmixed blessing for developing countries like ours. Do they really contribute to the economic stability and progress of the host countries? As a matter of fact, their utility lies in the field in which they are working. They must not be allowed to work in non-priority areas indiscriminately. In the recent years, external assistance to developing countries has been declining. This is because the donor developed countries have not been willing to part with a larger proportion of their GDP as assistance to developing countries. MNCs can bridge the gap between the requirements of foreign capital for increasing foreign investment in India.

In the case of India, foreign investment has flowed in non-priority areas in a significant proportion. Around 40% multinational companies in India are operating in sectors like hotels, tourism, food processing, service sector etc. There are very high rates of return in these sectors. Out of the total foreign investment in India by various countries, the share of USA alone is about 40%. Again, out of a total of 3700 collaborations, almost half of them are financial in nature. The result is that financial sector in India remains erratic.



Foreign investment in non-priority sectors has resulted in a new kind of consumerism in the form of colas, ice-creams, music systems, potato wafers, expensive bikes and cars. These items serve the need of only about 20% of population living in urban areas. On the other hand, the rest of the population is suffering from the lack of basic amenities. Again the portfolio investment in India is in the form of 'hot' money. This money can be easily diverted to their own countries. So, it is a mistake to treat portfolio investment as a stable factor. The increased Foreign Direct Investment (FDI) leads to inflationary trends. It is again a mistake to think that the entry of multinationals would ensure the transfer of high technology to India. There is no indication that technology is being transferred to the country. We just get the taste of screw driver technology. "India became the tenth-largest insurance market in the world in 2013, rising from 15th in 2011. At a total market size of US$66.4 billion in 2013, it remains small compared to world's major economies, and the Indian insurance market accounted for just 2% of the world's insurance business in 2017. India's life and non-life insurance industry collected 6.10 trillion (US$86 billion) in total gross insurance premiums in 2018. Life insurance accounts for 75.41% of the insurance market and the rest is general insurance. Of the 52 insurance companies in India, 24 are active in life-insurance business." (*BEF, Insurance Sector in India April 2014*)



At present multinational companies are operating in the areas where they get an excessively high rate of return. Take the example of Colgate Palmolive. Their rate of an return is estimated to be 80%. It is strange that we have not got a response from multinational companies engaged in oil production, power generation and other priority areas. They have, in fact, only made three solid contributions to our national economy. Firstly, they have used indigenous raw material instead of imports. Secondly, a cadre of professional managers has been trained. Thirdly, they have set up an efficient trading infrastructure.

"The information technology (IT) industry in India consists of two major components: IT Services and business process outsourcing (BPO). The sector has increased its contribution to India's GDP from 1.2% in 1998 to 7.5% in 2012.[293] According to NASSCOM, the sector aggregated revenues of US$147 billion in 2015, where export revenue stood at US$99 billion and domestic at US$48 billion, growing by over 13%." (*BEF, Insurance Industry in India*)

The investment in infrastructure will give a boost to industrial growth and help in creating income and employment in the India economy. The external economies generated by investment in infrastructure by MNCs will therefore crowd in investment by the indigenous private sector and will therefore stimulate economic growth. In view of above, even Common Minimum Programme of the present UPA government provides that foreign direct investment (FDI) will be encouraged and actively sought, especially in areas of (a) infrastructure, (b) high technology and (c) exports, and (d) where domestic assets and employment are created on a significant scale

Conclusion:

One can say that a multinational corporation is a mix of virtues and vices, boons and banes. Therefore, the government should adopt a pragmatic approach to them because multinationals have come to stay in the present day world. We will have to learn to live with multinationals under the new global economic order. Previously American based multinationals ruled the world, but today, many Japanese, Korean, European and Indian multinational companies have spread their wings in many parts of the world. Before entering into any country, at the headquarters of MNCs, experts from various fields such as political science, economics, commerce international trade and diplomacy are analyzing the business environment of a country and advising the top management.

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SCIENTOMETRIC ASSESSMENT OF CHEMICAL ENGINEERING LITERATURE AT GLOBAL LEVEL AS REFLECTED IN THE SCOPUS DATABASE FROM 2008 TO 2017

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Abstract

Using bibliographic records from the SCOPUS database, this paper attempts to give a complete view of evolution of the field of Chemical Engineering based on the literature published from 2008 to 2017.The study uses scientometric indicators such as Year-wise distribution, Relative growth rate of articles, doubling time, country-wise distribution, and applicability of the Bradford law in the field of chemical engineering is verified. The study is based on6993 articles published in the field of chemical engineering during the study period. The highest number of articles was published in the year 2017(974) and an average of 699 articles was published each year during the study period. The results of the study indicate that there is a declining trend in relative growth rate and an increasing trend in doubling the time of chemical literature over ten years. Canada is the most contributed country in the world(1023). The Bradford Law of scattering is not fitted in the field of chemical engineering. Finally, it can be concluded that significant research activity is taking place in the area of Chemical Engineering and it is one of the emerging research areas in the field of chemical sciences.

Keywords: Scientometrics, Chemical Engineering Literature, Relative Growth rate (RGR), Doubling Time(Dt), Geographical Distribution, Bradford Law.

1. INTRODUCTION

Historically, chemical engineering was largely an empirical and heuristic discipline, lacking quantitative, first□principles□based, modelling approaches. Chemical engineering is at an important crossroads. Our discipline is undergoing an unprecedented transition one that presents significant challenges and opportunities in modeling and automated decision□making. This has been driven by the convergence of cheap and powerful computing and communications platforms, tremendous progress in molecular engineering, the ever□increasing automation of globally integrated operations, tightening environmental constraints, and business demands for speedier delivery of goods and services to market. One important outcome from this convergence is the generation, use, and management of massive amounts of diverse data, information, and knowledge, and this is where AI, particularly ML, would play an important role.

Chemical engineering has developed as an important field of research mainly due to its role in drug discovery and for the chemical industry. It has always been an important area of research in chemical sciences in India. Besides the government-funded research agencies and academic institutions (universities and colleges), several privately funded R&D institutions in India are also involved in researching chemical engineering.

Scientometrics is a valuable technique for the evaluation of the research performance of a country or a group of countries or institutions and disciplines. Several scientometric studies dealing with different aspects of chemical engineering research in India have been reported in the literature.

Chemical engineering is the study and practice of transforming substances at large scales for the tangible improvement of the human condition. Such transformations are executed to produce other useful substances or energy, and lie at the heart of vast segments of the chemical for the benefit of society. In the present study, an attempt has been made to analyze and interpret the various dimensions of chemical engineering literature based on6996 records collected from the SCOPUS.

REVIEW OF LITERATURE:

Mahadevi R. Nyamagoudar and Gavisiddappa Anandhalli (2020). The paper reveals the growth of Chemistry literature for the period 2005-2016. A total of 24322 records were extracted from the Scopus Database for twelve years which is used as the main source of primary data for the present study. The growth models were applied to the literature of Chemistry. The result of the study indicates that the Relative Growth Rate (RGR) of the Chemistry publication was found to be a decreasing trend and Doubling Time (Dt) was found to be an increasing trend. The growth of literature in the field of Chemistry does not follow either a Polynomial or Power growth model. The study concluded that there has a consistent trend in the growth of Chemistry literature. The study can be concluded that chemical literature follows the moderately follows linear growth, Exponential growth, and Logistic growth model.

Neelamma and Gavisiddappa A(2016) have attempted to determine the materials cited in zoology literature during the year 2005–2014. The data were extracted from the Web of Science citation index database. The study reveals the distribution of citations for document type, language-wise distribution of citations, and country-wise distribution of citations. Further, the study also lists out the most productive journals in the area of zoology literature. The analysis of the results shows that out of 5332 citations, 74.81% of research articles contribute the highest number of citations and it is the most preferred source of information used by researchers in the area of zoology. The USA (33.75%) is the most cited country in the world and the English language (98.59%) is the most preferred language in the world. Bradford's law well fitted into the given data set for the present study. Finally, it can be concluded that significant research activity is taking place in the field of zoology and it is one of the emerging research fields in the biological sciences.

Neelamma and Anandhalli's (2016)present paper aims at analyzing the research output performance of Botany literature. Citation analysis of all the journal articles published in the Botany literature, which covered in Web of Science (on-line version database) from 2005 to 2014. A total of 12051 references were cited in 1183 articles in 572 journals. The study elaborates on various bibliometric components such as the distribution of citations for Document type, Language wise distribution of citations, and Country wise publication of citations. Further, the study also lists out the most productive journals in the field of Botany Literature. The analysis of the results shows that out of 12051 citations, Research articles (61.96%) contribute the highest number of citations and it is the most preferred source of information used by researchers in the field of Botany. The USA is the most cited country in the world and the English language is the most preferred language in the world. Bradford's law well fitted into the given data set for the present study. Finally, it can be concluded that significant research activity is taking place in the area of Botany and it is one of the emerging research fields in the biological sciences.

Sudhier Pillai (2010) has discussed scholarly contributions on the various facets of Bradford Law. In addition to the theoretical aspects of the law, papers dealing with the application of the law in the various subject fields. A study on five-year data of journals (2004–08) cited by the physicists at the Indian Institute of Science (IISC) Bangalore was carried out to examine the applicability of Bradford's laws of scattering, which includes 690 periodicals containing 11319 references collected from 79 doctoral theses during 2004–08. Ranked list of journals preferred, and physical review with 9.53% citations were the most preferred journals. The Bradford's multipliers were calculated and the law was found to be applicable with the value K as 1.2. The distribution of journals in three zones was made and the number of references in each zone was then estimated. The applicability of the Leimkuhler model was also tested with the present data.

Mahapatra (1994) has discussed the Relative Growth Rate (RGR) and Doubling time (Dt) for publications and citations which appeared in Indian Library and Information Science journals during 1975 - 1985 were determined. The reducing trend of RGR and increasing rate for doubling time in double-publications and citations indicates that the growth is neither exponential nor linear. The size of the literature is calculated by applying logistic growth formula, intellectual and environment conditions and with the increase of number of publications; the number of citations will also increase.

2. METHODOLOGY:

The dataset was collected from SCOPUS online database from 2008 to 2017. A total of 6993 articles were received for ten years. SCOPUS is one of the most comprehensive databases covering all subjects. The keyword ‘Chemical Engineering’ has been used for extracting the number of records available in the said database. Retrieved data were examined, classified, and analyzed keeping the objective in view. Further, the data is analyzed using MS-Excel spreadsheet and SPSS Software to test the formulated hypotheses at the beginning of the study.

3. OBJECTIVES OF THE STUDY:

The specific objectives of the study are.

1. To examine the relative growth rate and doubling time of chemical engineering literature as reflected in the SCOPUS.
2. To analyze the country-wise and form-wise distribution of literature in the field of chemical engineering
3. To identify the core journals in the field of Chemical Engineering &
4. To test the applicability of Bradford law of scattering in the field of chemical engineering.

Hypotheses.

1. There is a declining trend in relative growth rate and an increasing trend in doubling time of chemical engineering over ten years.
2. Bradford's law of scattering positively fitted with chemical engineering.

4. DATA ANALYSIS AND INTERPRETATION:

The study is based on 6993 articles published in the Scopus database over 10 years has been analyzed with a help of MS-Excel and SPSS software. Various statistical tools and Scientometrics indicators have been employed in the process of analysis and interpretation of data to draw a meaningful conclusion.

Table- 1Year Wise Growth Rate of World Chemical Engineering Literature from 2008 to 2017

Year	No of Records	% age	Cum Record	Cum %age	Growth rate	Descriptive Statistics	
2008	798	11.411	798	11.41		Average Growth	1.31
2009	242	3.461	1040	14.87	3.30	Mean	699.30
2010	865	12.370	1905	27.24	0.28	SD	271.198
2011	389	5.563	2294	32.80	2.22	MAX	974
2012	888	12.698	3182	45.50	0.44	MIN	242
2013	387	5.534	3569	51.04	2.29	Range	4.02479
2014	603	8.623	4172	59.66	0.64		
2015	902	12.899	5074	72.56	0.67		
2016	945	13.514	6019	86.07	0.95		
2017	974	13.928	6993	100.00	0.97		
	6993	**100**			**1.31**		

Table-1 depicts the growth of research publications published in the Scopus online database during the study period of 2008 to 2017. Altogether 6993 articles were published during the study period, the highest number of articles were contributed in the year 2017 (977), representing 13.928% of the total number of publications. The second-highest numbers of articles were published in the year 2016 (945). It is observed that the least number of articles were published in the year 2009 (242-3.461%), further it is observed that on average 699 articles were published per year during the study period with a standard deviation of 271 articles. It can be concluded that there is a consistently increasing trend in the growth of chemical engineering literature during the study period.

Table-2 Relative Growth Rate (RGR) and Doubling Time (DT) of Articles in Chemical Engineering from2008 to 2017

SI NO	Year	Quantum of output	Cumulative output	W1	W2	Rt(p)	Mean RP(p)	Dt(p)	Mean Dt(p)
1	2008	798	798	6.68	6.68	0.00	0.28	0.00	1.92
2	2009	242	1040	5.49	6.95	0.26		2.62	
3	2010	865	1905	6.76	7.55	0.61		1.14	
4	2011	389	2294	5.96	7.74	0.19		3.73	
5	2012	888	3182	6.79	8.07	0.33		2.12	
6	2013	387	3569	5.96	8.18	0.11	0.16	6.04	4.54
7	2014	603	4172	6.40	8.34	0.16		4.44	
8	2015	902	5074	6.80	8.53	0.20		3.54	
9	2016	945	6019	6.85	8.70	0.17		4.06	
10	2017	974	6993	6.88	8.85	0.15		4.62	
		6993							

Table-2 shows the relative growth rate and doubling time of articles in chemical engineering it is indicated that the value of relative growth rate of publications decreased from .28 in the year 2010 to .16 in the year 2017. Simultaneously the mean value of doubling time increased from 1.92 in the year 2009 to 4.54 in the year 2017. It is evident from the study that the research in the field of chemical engineering at the global level has increased over the period. It can be concluded that there is a declining trend in the relative growth rate of literature and an increasing trend in doubling the time of the article in chemical engineering during the study period.

Table- 3 Country-wise distribution of the literature

Rank	Name of the country	No of records	Cum no of records	Percent	Cum percentage
1	Canada	1023	1023	14.63	14.63
2	China	980	2003	14.01	28.64
3	United States	923	2926	13.20	41.84
4	India	571	3497	8.17	50.01
5	Iran	498	3995	7.12	57.13
6	United Kingdom	479	4474	6.85	63.98
7	Germany	425	4899	6.08	70.06
8	Japan	380	5279	5.43	75.49
9	South Korea	340	5619	4.86	80.35
10	France	267	5886	3.82	84.17
11	Spain	238	6124	3.40	87.57
12	Brazil	221	6345	3.16	90.73
13	Italy	203	6548	2.90	93.64
14	Czech Republic	176	6724	2.52	96.15
15	Australia	146	6870	2.09	98.24
16	Russian Federation	123	6993	1.76	100.00
		6993		**100**	

The geographical distribution of contribution is presented in the table-3 which gives the country-wise distribution of contribution of research output in the field of chemical engineering. Out of 6993 articles 1023 articles were published by Canada alone, which amounts to 14.63% of the total publications. Followed by China contributing 980 articles and U.S.A. Contributed 923 articles and India Contributed 571 articles, it is evident from the above table that the first four toped countries have made significant contribution i.e 50% to the total publications. Next followed by the United Kingdom 479, Germany 425, Japan 380, and South Korea 340 articles respectively. Therefore it can be concluded that Canada is the highest contributor in the field of chemical engineering at the global level and more than fifty percentage of the research contribution in the field of Chemical engineering is reported from the top four countries in the world, namely Canada, China, U.S.A and India and they are major contributors of chemical engineering literature at the global level.

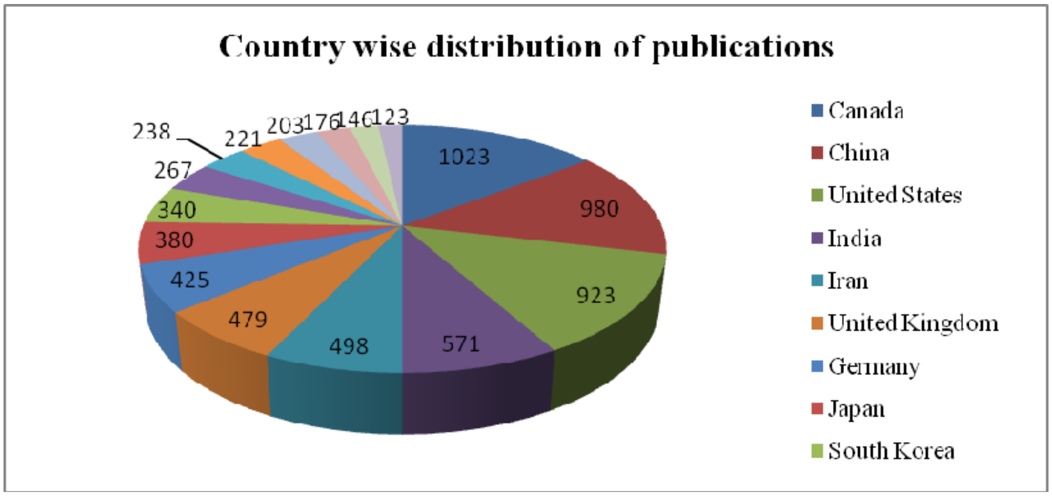
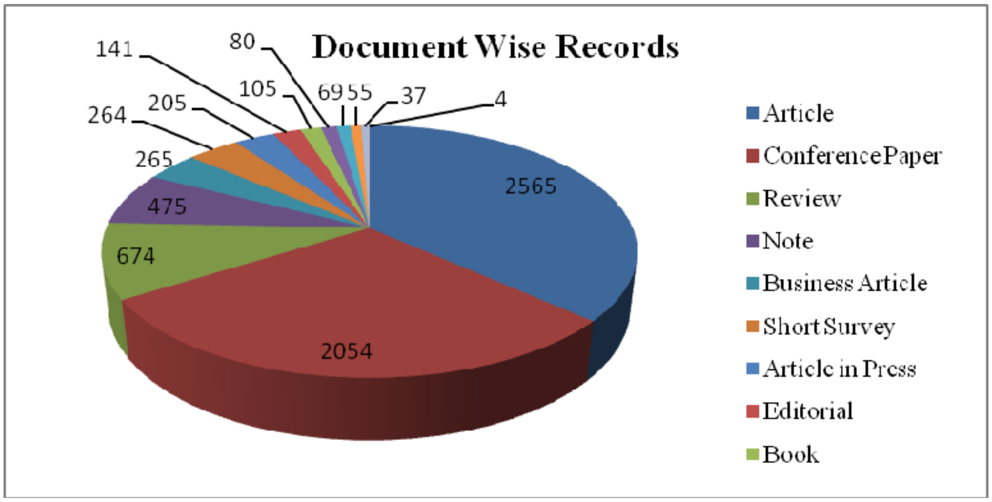


Table-4 Document Types wise Distribution of Articles

SI No	Type of documents	No of publications	Cum Articles	Percentage	Cum Percentage
1	Article	2565	2565	36.68	36.68
2	Conference Paper	2054	4619	29.37	66.05
3	Review	674	5293	9.64	75.69
4	Note	475	5768	6.79	82.48
5	Business Article	265	6033	3.79	86.27
6	Short Survey	264	6297	3.78	90.05
7	Article in Press	205	6502	2.93	92.98
8	Editorial	141	6643	2.02	94.99
9	Book	105	6748	1.50	96.50
10	Erratum	80	6828	1.14	97.64
11	Letter	69	6897	0.99	98.63
12	Book Chapter	55	6952	0.79	99.41
13	Conference Review	37	6989	0.53	99.94
14	Report	4	6993	0.06	100.00
		6993		**100**	

Table-4 shows document types of wise distribution of articles in the field of chemical engineering. It is evident from the table-4 that the highest number of publications published in the form of research articles which contributes alone 36.68 % to the total publications. The next highest number of publications published in the form of conference paper, which contributes nearly 29.37% and third-highest contribution of the publications in the form of Reviews, all these together contributes more than 75% to the total publications. Other is published in the form of Note, Business article, short survey, an article in press, editorial, book, and erratum. Therefore it can be concludedfrom the above analysis that research articles are the major mode of transmission of scholarly communication in the field of chemical engineering.



Ranking of Crystallography Journals:

There are numerous outlets to publish research work. Journal is one such significant medium through which the research papers can be published. The academic journals immensely contribute to the validation and the dissemination of breakthrough knowledge.

Journal rankings are the matrices that provide information on how a journal performs in comparison with other journals in the same field.

Ranking of Chemical Engineering Journals:

Based on the contribution of several articles contributed by each journal the ranking has been given. Based on the productivity the ranking has been done.

The table-5 Core journals in the field of Chemical Engineering

Rank	Journal Name	No of Articles	Cum No of Article	% Age	Cum%age
1	Canadian Journal Of Chemical Engineering	1851	1851	26.469	26.469
2	Journal Of Industrial And Engineering Chemistry	860	2711	12.298	38.767
3	HuaxueGongcheng Chemical Engineering China	571	3282	8.165	46.933
4	Gao Xiao Hua Xue Gong Cheng XueBao Journal Of Chemical Engineering Of Chinese Universities	417	3699	5.963	52.896
5	Chemical Engineering Transactions	308	4007	4.404	57.300
6	Chemical And Engineering News	230	4237	3.289	60.589
7	ACS Catalysis	135	4372	1.931	62.520
8	Powder Technology	91	4463	1.301	63.821
9	XiandaiHuagong Modern Chemical Industry	68	4531	0.972	64.793
10	International Journal Of Chemical Reactor Engineering	37	4568	0.529	65.322
11	Applied Catalysis A General	31	4599	0.443	65.766
12	Colloids And Surfaces A Physicochemical And Engineering Aspects	29	4628	0.415	66.180
13	Kobunshi	29	4657	0.415	66.595
14	Dyes And Pigments	28	4685	0.400	66.996
15	Chinese Journal Of Chemical Engineering	27	4712	0.386	67.382
16	Chemical Engineer	19	4731	0.272	67.653
17	Reviews In Chemical Engineering	18	4749	0.257	67.911
18	Chemical Engineering Science	17	4766	0.243	68.154
19	Transport In Porous Media	17	4783	0.243	68.397
20	Brazilian Journal Of Chemical Engineering	15	4798	0.215	68.611
21	Indian Chemical Engineer	13	4811	0.186	68.797
22	Particulate Science And Technology	13	4824	0.186	68.983
23	Catalysis Science And Technology	12	4836	0.172	69.155
24	Frontiers Of Chemical Science And Engineering	11	4847	0.157	69.312
25	Hydrocarbon Engineering	10	4857	0.143	69.455
26	International Journal Of Chemical Engineering	10	4867	0.143	69.598
27	Neural Regeneration Research	10	4877	0.143	69.741
28	PeriodicaPolytechnica Chemical Engineering	8	4885	0.114	69.856
29	Beijing	7	4892	0.100	69.956

	HuagongDaxueXuebaoZiranKexueban Journal Of Beijing University Of Chemical Technology Natural Science Edition				
30	Process Engineering	7	4899	0.100	70.056
31	Trends In Biotechnology	7	4906	0.100	70.156
32	Chemical Week	6	4912	0.086	70.242
33	China Petroleum Processing And Petrochemical Technology	6	4918	0.086	70.327
34	Recent Patents On Chemical Engineering	6	4924	0.086	70.413
35	Revista Mexicana De IngenieraQumica	6	4930	0.086	70.499
36	Atomization And Sprays	5	4935	0.072	70.571
37	Catalysis In Industry	5	4940	0.072	70.642
38	Chemical Industry And Chemical Engineering Quarterly	5	4945	0.072	70.714
39	Journal Of Thermal Analysis And Calorimetry	5	4950	0.072	70.785
40	Korean Chemical Engineering Research	5	4955	0.072	70.857
41	Process Engineering London	5	4960	0.072	70.928
42	Process Systems Engineering	5	4965	0.072	71.000
43	Recent Innovations In Chemical Engineering	5	4970	0.072	71.071
44	Chemical Engineering Progress	4	4974	0.057	71.128
45	Journal Of Chemical Engineering Of Japan	4	4978	0.057	71.185
46	Journal Of Neuroscience	4	4982	0.057	71.243
47	Progress In Brain Research	4	4986	0.057	71.300
48	Bioengineering Proceedings Of The Northeast Conference	3	4989	0.043	71.343
49	Bulletin Of Chemical Reaction Engineering And Catalysis	3	4992	0.043	71.386
50	Chemical Engineering	3	4995	0.043	71.429
51	Desalination	3	4998	0.043	71.471
52	International Paperworld IPW	3	5001	0.043	71.514
53	Kami Pa Gikyoshi Japan Tappi Journal	3	5004	0.043	71.557
54	Neuron	3	5007	0.043	71.600
55	Revista Mexicana De IngenieraQuimica	3	5010	0.043	71.643
56	CIT Plus	2	5012	0.029	71.672
57	Catalysis Today	2	5014	0.029	71.700
58	Chemical Engineering Communications	2	5016	0.029	71.729

59	Current Opinion In Neurobiology	2	5018	0.029	71.757
60	Frontiers Of Chemical Engineering In China	2	5020	0.029	71.786
61	HuagongXuebao Journal Of Chemical Industry And Engineering China	2	5022	0.029	71.815
62	Molecular Neurobiology	2	5024	0.029	71.843
63	Nature Neuroscience	2	5026	0.029	71.872
64	Neuroscience Letters	2	5028	0.029	71.900
65	Open Chemical Engineering Journal	2	5030	0.029	71.929
66	Petroleum Technology Quarterly	2	5032	0.029	71.958
67	Sheng Wu Yi Xue Gong Cheng XueZaZhi Journal Of Biomedical Engineering ShengwuYixueGongchengxueZazhi	2	5034	0.029	71.986
68	Thermal Science And Engineering Progress	2	5036	0.029	72.015
69	Applied Chemistry For Engineering	1	5037	0.014	72.029
70	Behavioral Neuroscience	1	5038	0.014	72.043
71	Biological Psychiatry	1	5039	0.014	72.058
72	Bulletin Of Chemical Reaction Engineering Catalysis	1	5040	0.014	72.072
73	Catalysis Communications	1	5041	0.014	72.086
74	Chemical Engineering And Processing Process Intensification	1	5042	0.014	72.101
75	Chemical Processing	1	5043	0.014	72.115
76	Chemosensory Perception	1	5044	0.014	72.129
77	Chung KuoTsaoChih China Pulp And Paper	1	5045	0.014	72.144
78	CuihuaXuebao Chinese Journal Of Catalysis	1	5046	0.014	72.158
79	Current Protocols In Neuroscience	1	5047	0.014	72.172
80	European Journal Of Neuroscience	1	5048	0.014	72.186
81	Experimental Neurology	1	5049	0.014	72.201
82	Explosion	1	5050	0.014	72.215
83	Filtration And Separation	1	5051	0.014	72.229
84	Frontiers In Cellular Neuroscience	1	5052	0.014	72.244
85	Frontiers In Neuroscience	1	5053	0.014	72.258
86	Others	1940	6993	27.742	100.000
	Total	**6993**		100	

Table -5 shows the most productive journals in the field of chemical engineering, it is observed that the top four journals namely Canadian Journal Of Chemical Engineering (1851), Journal Of Industrial And Engineering Chemistry (860), Huaxue Gongcheng

Chemical Engineering China (571) and Gao Xiao Hua Xue Gong Cheng XueBao Journal Of Chemical Engineering Of Chinese Universities (417) are core journals in the field of chemical engineering contributed more than 50% to the total publications at the global level.

Application of Bradford Law

According to S C Bradford, the papers relevant to the subject field may be divided into three successive zones, each producing $(1/3)^{rd}$ of the total relevant papers. If the scientific journals are arranged in the order of decreasing productivity of articles on a given subject.

For the present study Leimkuhler's (1967) equation has been applied to study the Broadford distribution.

$$F(x) = \frac{\log(1+Bx)}{\log(1+B)}$$

Where B is connected with x as

$$X=\frac{1}{\log(1+Bx)}-\frac{1}{B}$$

Where $X=\frac{if(f)}{n}$

The equation of $E(X)=\frac{\log(1+Bx)}{\log(1+B)}$

Can be written as

$$\overline{X}=\frac{1}{\log(1+B)}+\frac{1}{B}$$

With the help of $\overline{X}$ value the B value is calculated by using trial and error method

B=59.46 , X = .5896

F= Frequency Distribution
F(X) = Observed value
If (I)= Frequency Calculation
FX=Bradford's Theoretical Distribution
E(x) = Expected Value
Diff=Difference of observed value and expected value.
The absolute tabulated value=**0.274715**
The absolute calculated value=**0.175767**

Hypothesis : The distribution of publications in the field of Chemical Engineering follows the Bradford law of scattering

Table-6 Parameter value for Bradford distribution in Chemical Engineering

Rank	No of Articles	Cum	X	f(i)	F(x)	if(I)	E(X)	D
1	1851	1851	0.011628	0.264693	0.264693	0.003078	0.13964	0.125053
2	860	2711	0.023256	0.12298	0.387673	0.009016	0.226582	0.161091
3	571	3282	0.034884	0.081653	0.469326	0.016372	0.289876	0.17945
4	417	3699	0.046512	0.059631	0.528958	0.024603	0.339673	0.189285
5	308	4007	0.05814	0.044044	0.573002	0.033314	0.38073	0.192272
6	230	4237	0.069767	0.03289	0.605892	0.042272	0.415661	0.190231
7	135	4372	0.081395	0.019305	0.625197	0.050888	0.446059	0.179137
8	91	4463	0.093023	0.013013	0.63821	0.059368	0.472967	0.165242
9	68	4531	0.104651	0.009724	0.647934	0.067807	0.497105	0.150829
10	37	4568	0.116279	0.005291	0.653225	0.075956	0.518989	0.134236
11	31	4599	0.127907	0.004433	0.657658	0.084119	0.539005	0.118652
12	29	4628	0.139535	0.004147	0.661805	0.092345	0.557448	0.104357
13	29	4657	0.151163	0.004147	0.665952	0.100667	0.574545	0.091406
14	28	4685	0.162791	0.004004	0.669956	0.109063	0.590481	0.079474
15	27	4712	0.174419	0.003861	0.673817	0.117526	0.605403	0.068413
16	19	4731	0.186047	0.002717	0.676534	0.125867	0.619433	0.057101
17	18	4749	0.197674	0.002574	0.679108	0.134242	0.632671	0.046437
18	17	4766	0.209302	0.002431	0.681539	0.142648	0.645202	0.036337
19	17	4783	0.22093	0.002431	0.68397	0.15111	0.657097	0.026873
20	15	4798	0.232558	0.002145	0.686115	0.159562	0.668418	0.017696
21	13	4811	0.244186	0.001859	0.687974	0.167994	0.679218	0.008755
22	13	4824	0.255814	0.001859	0.689833	0.176469	0.689543	0.00029
23	12	4836	0.267442	0.001716	0.691549	0.184949	0.699433	0.007884
24	11	4847	0.27907	0.001573	0.693122	0.193429	0.708922	0.015801
25	10	4857	0.290698	0.00143	0.694552	0.201905	0.718043	0.023491
26	10	4867	0.302326	0.00143	0.695982	0.210413	0.726822	0.030841
27	10	4877	0.313953	0.00143	0.697412	0.218955	0.735285	0.037873
28	8	4885	0.325581	0.001144	0.698556	0.227437	0.743453	0.044897
29	7	4892	0.337209	0.001001	0.699557	0.235897	0.751346	0.051789

30	7	4899	0.348837	0.001001	0.700558	0.244381	0.758982	0.058425
31	7	4906	0.360465	0.001001	0.701559	0.252887	0.766378	0.064819
32	6	4912	0.372093	0.000858	0.702417	0.261364	0.773548	0.071131
33	6	4918	0.383721	0.000858	0.703275	0.269861	0.780505	0.07723
34	6	4924	0.395349	0.000858	0.704133	0.278378	0.787261	0.083129
35	6	4930	0.406977	0.000858	0.704991	0.286915	0.793829	0.088838
36	5	4935	0.418605	0.000715	0.705706	0.295412	0.800218	0.094512
37	5	4940	0.430233	0.000715	0.706421	0.303925	0.806437	0.100016
38	5	4945	0.44186	0.000715	0.707136	0.312455	0.812496	0.10536
39	5	4950	0.453488	0.000715	0.707851	0.321002	0.818402	0.110551
40	5	4955	0.465116	0.000715	0.708566	0.329565	0.824163	0.115598
41	5	4960	0.476744	0.000715	0.709281	0.338145	0.829786	0.120506
42	5	4965	0.488372	0.000715	0.709996	0.346742	0.835278	0.125282
43	5	4970	0.5	0.000715	0.710711	0.355355	0.840644	0.129933
44	4	4974	0.511628	0.000572	0.711283	0.363912	0.84589	0.134607
45	4	4978	0.523256	0.000572	0.711855	0.372482	0.851021	0.139166
46	4	4982	0.534884	0.000572	0.712427	0.381065	0.856043	0.143616
47	4	4986	0.546512	0.000572	0.712999	0.389662	0.860959	0.14796
48	3	4989	0.55814	0.000429	0.713428	0.398192	0.865774	0.152346
49	3	4992	0.569767	0.000429	0.713857	0.406732	0.870493	0.156636
50	3	4995	0.581395	0.000429	0.714286	0.415282	0.875118	0.160832
51	3	4998	0.593023	0.000429	0.714715	0.423842	0.879654	0.164939
52	3	5001	0.604651	0.000429	0.715144	0.432412	0.884104	0.16896
53	3	5004	0.616279	0.000429	0.715573	0.440992	0.888471	0.172899
54	3	5007	0.627907	0.000429	0.716002	0.449582	0.892759	0.176757
55	3	5010	0.639535	0.000429	0.716431	0.458182	0.896969	0.180538
56	2	5012	0.651163	0.000286	0.716717	0.466699	0.901105	0.184389
57	2	5014	0.662791	0.000286	0.717003	0.475223	0.90517	0.188167
58	2	5016	0.674419	0.000286	0.717289	0.483753	0.909165	0.191877
59	2	5018	0.686047	0.000286	0.717575	0.49229	0.913094	0.195519
60	2	5020	0.697674	0.000286	0.717861	0.500833	0.916958	0.199097
61	2	5022	0.709302	0.000286	0.718147	0.509383	0.920759	0.202612

62	2	5024	0.72093	0.000286	0.718433	0.51794	0.924499	0.206067
63	2	5026	0.732558	0.000286	0.718719	0.526503	0.928181	0.209463
64	2	5028	0.744186	0.000286	0.719005	0.535073	0.931806	0.212802
65	2	5030	0.755814	0.000286	0.719291	0.54365	0.935376	0.216085
66	2	5032	0.767442	0.000286	0.719577	0.552233	0.938893	0.219316
67	2	5034	0.77907	0.000286	0.719863	0.560823	0.942357	0.222494
68	2	5036	0.790698	0.000286	0.720149	0.56942	0.945771	0.225622
69	1	5037	0.802326	0.000143	0.720292	0.577908	0.949136	0.228844
70	1	5038	0.813953	0.000143	0.720435	0.5864	0.952454	0.232019
71	1	5039	0.825581	0.000143	0.720578	0.594896	0.955725	0.235147
72	1	5040	0.837209	0.000143	0.720721	0.603394	0.958951	0.23823
73	1	5041	0.848837	0.000143	0.720864	0.611896	0.962134	0.24127
74	1	5042	0.860465	0.000143	0.721007	0.620401	0.965273	0.244267
75	1	5043	0.872093	0.000143	0.72115	0.62891	0.968372	0.247222
76	1	5044	0.883721	0.000143	0.721293	0.637421	0.97143	0.250137
77	1	5045	0.895349	0.000143	0.721436	0.645937	0.974449	0.253013
78	1	5046	0.906977	0.000143	0.721579	0.654455	0.977429	0.25585
79	1	5047	0.918605	0.000143	0.721722	0.662977	0.980372	0.25865
80	1	5048	0.930233	0.000143	0.721865	0.671502	0.983279	0.261414
81	1	5049	0.94186	0.000143	0.722008	0.680031	0.98615	0.264142
82	1	5050	0.953488	0.000143	0.722151	0.688562	0.988986	0.266835
83	1	5051	0.965116	0.000143	0.722294	0.697097	0.991788	0.269494
84	1	5052	0.976744	0.000143	0.722437	0.705636	0.994558	0.272121
85	1	5053	0.988372	0.000143	0.72258	0.714178	0.997295	0.274715
86	1940	6993	1	0.27742	1	1	1	0
	6993				59.43372	31.26142	0	**0.274715**

Test of exponentiality of distribution of articles

Kalmogorov Simonov test (K-S test) is applied to test the exponentiality of the distribution by using the formula.

$$E(X)=1-e^{\theta x}$$

Where $\theta = \frac{1}{\bar{x}}$

X=1,2,3,4..........n

The estimated values are presented in column 8 in the table-6

According to this test, the maximum deviation is observed and the estimated value Dmax value is calculated as follows

Dmax=F(x) – E(x). =0.274715

At the 0.01 level of significance, the KS statistics is equal to $\frac{1.63}{\sqrt{n}}$= if D is greater than KS-statistics than the distribution does not follow theoretical distribution at this level of significance, in this case, n=86, hence the KS statistics for the .01 level should be $\frac{1.63}{\sqrt{86}}$=0.175767. Since, the maximum difference value (.274715) is more than KS-statistics value (.175767), hence the given data set does fit into the given distribution, therefore, it can be concluded that with help of KS statistics "**The distribution of publications in the field of Chemical Engineering does not follow the Bradford law of scattering".** Hence the null hypothesis is rejected and the alternative hypothesis is accepted.

CONCLUSION:

The bibliometric techniques are the most powerful tool used for quantitative analysis, in the present study an attempt was made to analyze the various bibliometric dimensions and examination of Bradford law by using Leimkuhler's model in the field of chemical engineering. The study is based on 6996 research articles published from 2008 to 2017 as reflected in the Scopus database which is one of the most comprehensive databases. The study reveals the various bibliometric indicators like year-wise distribution, doubling time and relative growth rate of publications and country-wise distribution, documents type wise and identification of core list of journals and examination of Bradford law in chemical engineering. The results of the present study show that there is a consistent growth of publication in the field of chemical engineering. There is a declining trend inthe relative growth rate of publication and an increasing trend in doubling the time of articles over some time. Research articles are the major mode of transmission of scholarly communication in the field of chemical engineering. Canada is the highest contributor in the field of chemical engineering at the global level and fifty percentage of the research contribution in the field of Chemical engineering contributed by Canada, China, Germany, and India. Further, it is found that the Canadian Journal of Chemical Engineering, Journal of Industrial And Engineering Chemistry, and HuaxueGongcheng Chemical Engineering China are the top core journals in the field of chemical engineering. The Bradford law of scattering is not well fitted and followed in the field of chemical engineering which is confirmed with Leimkuhler's model.

Finally, it can be concluded that there has been a consistent trend towards increasing percentage of growth of publications in the field of chemical engineering and it is one of the most emerging areas in the field of chemical sciences.

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Library Philosophy and Practice (e-journal)
Libraries at University of Nebraska-Lincoln

Winter 1-8-2021

An Evaluation of the Indian Chemical Science Research Publications Output of the Last Two Decades (2000 – 2019)

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NYAMAGOUDAR, MAHADEVI and Anandhalli, Gavisiddappa, "An Evaluation of the Indian Chemical Science Research Publications Output of the Last Two Decades (2000 – 2019)" (2021). *Library Philosophy and Practice (e-journal)*. 4931.
https://digitalcommons.unl.edu/libphilprac/4931

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ABSTRACT

This study evaluates the Indian chemical science research output of the last two decades (2000 to 2019). We have made a scientometric analysis of contributions from India in leading chemical science journals over 20 years period 2000 – 2019. We have compared India's performance with that of the USA. The data was sourced from the Scopus database during 2000 – 19. The study finds that the research output of the world in chemical science research was 76, 08,260 publications and it was 469,689 publications by India, accounting for 6.1% global publications share in a 20 years window covering the period 2000-2019. The *USA with a highest of 1665017publications on World Chemical Science research, followed by China with 1598167 (21.010%) publications, the highest number of papers published in the subject area is Chemistry 11, 65,377 publications followed by Materials Science 1,19,949, RSC Advances journal from the United Kingdom published the highest publications i.e. 6,578 articles (6.609%) followed by Research Journal Of Pharmaceutical Biological And Chemical Sciences (India) published 4,192 (4.212%) articles, Indian Institute of Science, Bengaluru contributed the highest publications to the field of chemical science i.e. 15510 (3.537%).*

Keywords: Chemical Science, India, Evaluation, Research publications, Scopus, Scientometrics.

1. Introduction

Chemistry is one of the oldest of science and also one of the newest of science, without which modern life would not have been possible. Chemistry subject has grown from a study of some twenty-odd elements in the eighteenth century to a study of bonding between atoms in the 1950s, ad further on to investigations on structure, synthesis, dynamics, catalysis and supramolecular assemblies and today to photochemistry. Today major frontiers of chemistry relate to biology and advanced materials, chemistry has overlap regions with several other disciplines, which make for diverse applications of science for humanity. Evaluation of Indian chemical science research would help in assessing India's contribution to world literature in chemical science. Such an exercise, based on published literature, has already been made by many groups in developed countries. However, such studies as applied to third world countries are rather limited.

The evaluation of research performance of a country, a region, research and academic institutions, discipline, etc can be effectively done with scientometric techniques. Scientometrics presents a unique set of techniques for the monitoring, evaluation and analysis of information resources and the management of knowledge. These studies are being conducted to assess the quantitative and qualitative development of different subjects and disciplines, especially in the sciences. Chemical science research and development have brought out several studies. Hence, to assess the quantitative developments in the field of chemical science research using scientometric methods are useful to the stakeholders of this field of knowledge. The present study investigates various characteristics of research productivity in chemical science from India covered in Scopus.

The literature review summarizes and highlights the related papers on present research scenario of Science and technology in India as well as in the field of chemical science with sub discipline.

(Karki & Garg, 1999) assessed the performance of Indian organic chemistry research during the 70s and 80s. Identifies the significant work and its impact using mainstream connectivity, surrogate measures of quality and relative impact indicators. (Kaygusuz, 2019) evaluated chemistry research in 51 different European countries between years 2006 and 2016 was studied using statistical methods. (Fu, Long, & Ho, 2014) evaluate China's scientific output of chemical engineering in Science Citation Index Expanded in the Web of Science from 1992 to 2011. (Sudhier & Dileepkumar, 2020) examines 25,132 biochemistry research contributions of Indian scientists covered in the Web of Science for a period of 10 years (2004-2013). (Chaman Sab, Dharani Kumar, & Biradar, 2019) Indian publications output in marketing research during 1990-2018 on several parameters including contribution and citation impact of most productive countries, India's overall contribution, its growth pattern, citation impact, the share of international collaboration, identification of significant participating countries in India's international collaboration, most productivity and impact of leading Indian institutions and authors. (Hosamani,S C & Vitthal, 2019) Identified analyses the contributions of Indian chemistry literature in publishing research papers as reflected in Thomson Reuters, Web of Science database. (Mallikarjun, B., Kappi, 2020) Examined Asthma has become very essential, thus the purpose of the study was to map and analyse the trends by using scientometric tools to the Asthma literature published between 2010 and 2019. (Chaman Sab, Kappi, Bagalkoti, & Biradar, 2020) analysed bibliometric analysis of Indian Journal of Marketing. This journal is a double blind peer reviewed refereed monthly journal, which is being published since 1968. (Sudhier & Dileepkumar, 2020) examines 25,132 biochemistry research contributions of Indian scientists covered in the Web of Science for a period of 10 years (2004-2013). (Chaman Sab, Kumar; & Biradar, 2009) evaluated to qualitative analyse of medicine research output using select scientometric indicators with the aim of identifying top preparing countries, subject subthemes, organisations, authors and journals in the area.

2. Scope of the Study

Now, the scope of the research is limited to studies published by the Indian Chemical Science literature output during 2000 – 2019, listed in the Scopus database. The research area was limited to 20 years i.e., 2000-2019. The study was evaluated all publications in the Scopus database, irrespective of type or category.

3. Objectives of the Study

The study analysed Chemical Science research output by India with the Scopus database during 2000 – 2019 for evaluating research performance. The study will focus on (i) distribution of research publications by document type and source publications type; (ii) annual and cumulative growth in the subject, publication impact of the publications output and distribution of international collaborative papers by countries in collaborative research with India; (iii) Profile of top 50 most productive countries in the world in the subject; (iv) distribution of research publications by broad subject areas; (v) profile top 50 organisations and authors by publication output; (vi) identify important channels of research communications; describe characteristics of high cited papers in the subject.

4. Methodology

The Scopus is a global online bibliographic information base that is distributed and kept up by Elsevier and it is accessible by the membership. The Indian chemical science research publications published during 2000 – 2019 were studied. Keywords used for publications ALL(Chemical Science) AND PUBYEAR > 1999 AND PUBYEAR < 2020 AND (LIMIT-TO (AFFILCOUNTRY,"India")) A sum of 469,689. These records from India and 7,608,260 records from the world and the information were organized in MS Excel.

5. Analysis and results

5.1. Publications growth analysis

As seen from the Scopus database, the total research output of the world in chemical science research was 76, 08,260 publications and it was 469,689 publications by India, accounting for 6.1% global publications share in a 20 years window covering the period 2000-2019. Table 1 reveals that the Indian Chemical Science Literature along with cumulative output from 2000 to 2019. It is absorbed that 20 years study period, a total of 469689 publications are published. Out of 20 years, the year 2019 was most productive with 49,978 (10.64%) publications, followed by 46,726 (9.94%) in the year 2018, 42,592 (9.06%) in the year 2017 and the least number of 5,556 (1.18%) publications in the year 2000. The compound annual growth rate is 8.325%. The average research publication per year is 23484.45; the overall study period of 20 years is categorized into five segments of block years. In which the last block year of 2015-2019 responsible for the maximum of 2,206,717 (46.95%) publications on Indian Chemical Science research, followed by the block year of 2010-2014 with 146,999 (31.27%) publications and the block year of 2005-2009 with 66,403 (14.11%) publications.

Table 1: Indian Research output in Chemical Sciences research

Year	TP	TP Share (%)	Cumulative	Cumulative %
2000	5556	1.18	5556	1.183
2001	6356	1.35	11912	2.536
2002	7363	1.56	19275	4.104
2003	8070	1.71	27345	5.822
2004	8325	1.77	35670	7.594
2005	9973	2.12	45643	9.718
2006	11484	2.44	57127	12.163
2007	12975	2.76	70102	14.925
2008	14644	3.11	84746	18.043
2009	17327	3.68	102073	21.732
2010	20955	4.46	123028	26.194
2011	26628	5.66	149656	31.863
2012	29440	6.26	179096	38.131
2013	32412	6.9	211508	45.031
2014	37564	7.99	249072	53.029
2015	39317	8.37	288389	61.4
2016	42004	8.94	330393	70.343
2017	42592	9.06	372985	79.411
2018	46726	9.94	419711	89.359
2019	49978	10.64	469689	100
2000 – 2004	**35670**	**7.57**	**35670**	**7.57**
2005 – 2009	**66403**	**14.11**	**102073**	**21.68**
2010 – 2014	**146999**	**31.27**	**249072**	**52.95**
2015 – 2019	**2206717**	**46.95**	**2455789**	**100**

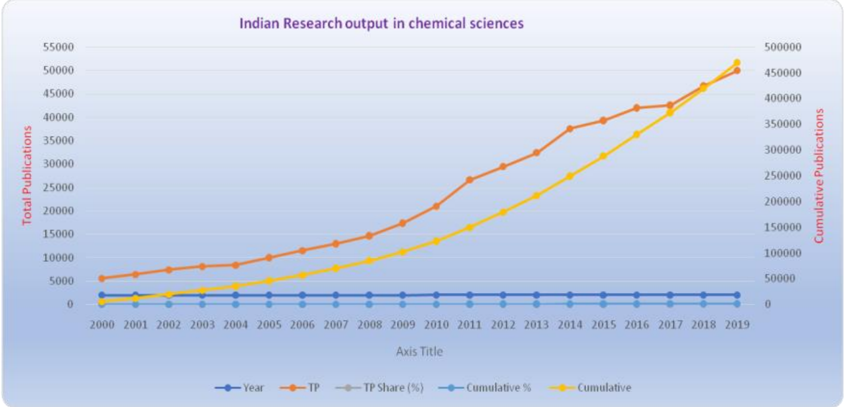

Fig. 1: Status of Indian Chemical Science Literature

5.2. Chemical Science publications of World and India versus Block Year

Table 2 and figure 2 shows that the overall study period of 20 years is categorized into five segments of block years. In which the last block year of 2016-2019 responsible for the maximum of 2,453,501 (32.254%) publications on World Chemical Science research, followed by the block year of 2012-2015 with 1,960,735 (25.776%) publications and the block year of 2008-2011with 1,426,015(18.747%) publications.

Table 2: Chemical Science of World Research versus Block Year

Sl No	Block Year	NP	%	CP	%
1	2000-2003	744321	9.785	744321	9.785
2	2004-2007	1022142	13.437	1766463	23.222
3	2008-2011	1426015	18.747	3192478	41.969
4	2012-2015	1960735	25.776	5153213	67.746
5	2016-2019	2453501	32.254	7606714	100.000
		7606714	**100**		

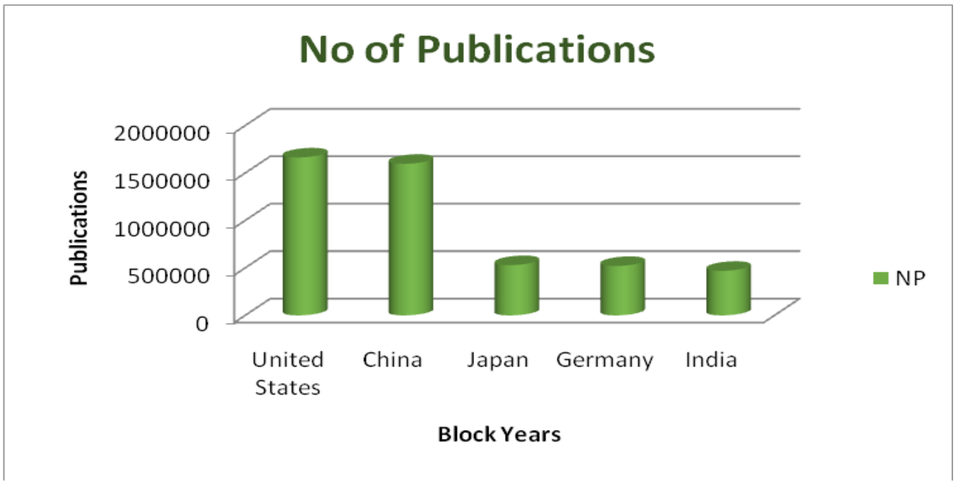

Fig. 2: Chemical Science of World Research versus Block Year

5.3. Country-wise Growth of Publications

Country-wise research publications of World Chemical Science have been analysed the top 50 countries based on research. Table 3 shows that the country-wise total number of publications, percentage and rank are calculated during the 20 years study period. It is identified that more than one-fifth of research publications are contributed by the USA (21.889%) and China (21.010%). The USA with the highest of 1,665,017publications on World Chemical Science research, followed by China with 1598167 (21.010%) publications, Japan with 529,834 (6.965%) publications, Germany with 521,234 (6.852%) publications, and India with 469,671(6.174%) publications. It is found that a total of 159 countries are involved in the 9,969,216 publications during the study. Among these, 62.891% of publications are published by the top five countries viz. the USA, China, Japan, Germany and India.

Table 3: Country-Wise Ranking

Sl. No	Country	NP	%	Rank
1	United States	1665017	21.889	1
2	China	1598167	21.010	2
3	Japan	529834	6.965	3
4	Germany	521234	6.852	4
5	India	469671	6.174	5
6	United Kingdom	428530	5.634	6
7	France	359833	4.730	7
8	South Korea	280407	3.686	8
9	Italy	278206	3.657	9
10	Canada	261882	3.443	10
11	Spain	251250	3.303	11
12	Russian Federation	233729	3.073	12
13	Australia	205123	2.697	13
14	Brazil	181448	2.385	14
15	Iran	160676	2.112	15
16	Poland	140233	1.844	16
17	Netherlands	127916	1.682	17
18	Taiwan	127032	1.670	18
19	Switzerland	120879	1.589	19
20	Sweden	111399	1.464	20
21	Turkey	106134	1.395	21
22	Belgium	88320	1.161	22
23	Malaysia	78726	1.035	23
24	Egypt	70337	0.925	24
25	Czech Republic	68819	0.905	25
26	Mexico	66510	0.874	26
27	Portugal	66229	0.871	27
28	Denmark	65735	0.864	28
29	Singapore	64124	0.843	29
30	Austria	62589	0.823	30
31	Saudi Arabia	62314	0.819	31

32	Israel	54986	0.723	32
33	Hong Kong	54123	0.712	33
34	Finland	54037	0.710	34
35	Greece	50516	0.664	35
36	South Africa	47573	0.625	36
37	Pakistan	47481	0.624	37
38	Thailand	44975	0.591	38
39	Norway	44561	0.586	39
40	Argentina	42641	0.561	40
41	Romania	38723	0.509	41
42	Hungary	38152	0.502	42
43	Ukraine	37920	0.499	43
44	New Zealand	35395	0.465	44
45	Ireland	33910	0.446	45
46	Indonesia	28561	0.375	46
47	Chile	26374	0.347	47
48	Nigeria	23277	0.306	48
49	Serbia	22419	0.295	49
50	Slovakia	21873	0.288	50

5.4. High Productive Subject Areas in chemical science Literature (India).

Table - 4 shows that Chemistry, Materials Science and Physics and Astronomy are the three high priority research areas of chemical science Literature with each contributing publication share 17.670%, 12.816% and 10.499% in the national publication output during 2000-2019. The highest number of papers published subject area is Chemistry 11,65,377 publications followed by Materials Science 1,19,949 research papers, Physics and Astronomy published 98,267 research papers, Biochemistry, Genetics and Molecular Biology published 85,699 research papers, Engineering published 83,164 research papers, Chemical Engineering published 74,929 papers, Pharmacology, Toxicology and Pharmaceutics published 65,636 papers, Agricultural and Biological Sciences published 50,376 papers, Environmental Science published 49,409 papers, Medicine published 30,344 papers, Energy published 24,363 papers, Immunology and Microbiology published 15,352 papers, Computer Science published 15,279 papers, Earth and Planetary Sciences published 14,817 papers, Mathematics published 11,447 papers and remaining 13 subject areas published below 1%.

Table 4: Most Preferred Subject/ Research Areas

SN	Subject Areas	TP	%
1	Chemistry	165377	17.670
2	Materials Science	119949	12.816
3	Physics and Astronomy	98267	10.499
4	Biochemistry, Genetics and Molecular Biology	85699	9.157
5	Engineering	83164	8.886
6	Chemical Engineering	74929	8.006
7	Pharmacology, Toxicology and Pharmaceutics	65636	7.013
8	Agricultural and Biological Sciences	50376	5.382
9	Environmental Science	49409	5.279
10	Medicine	30344	3.242
11	Energy	24363	2.603
12	Immunology and Microbiology	15352	1.640
13	Computer Science	15279	1.633
14	Earth and Planetary Sciences	14817	1.583
15	Mathematics	11447	1.223
16	Multidisciplinary	8962	0.958
17	Social Sciences	4245	0.454
18	Business, Management and Accounting	3287	0.351
19	Veterinary	2689	0.287
20	Economics, Econometrics and Finance	2641	0.282
21	Neuroscience	2632	0.281
22	Health Professions	1985	0.212
23	Nursing	1532	0.164
24	Decision Sciences	1160	0.124
25	Dentistry	1109	0.118
26	Psychology	848	0.091
27	Arts and Humanities	423	0.045
28	Undefined	3	0.000
		935924	100.000

5.5. Source wise distribution of Indian contributions in chemical science literature

The topmost productive journals publishing India’s research papers in chemical science research contributed 99,531 papers, which accounts for a 39.17% share in the cumulative publications output of India from 2000 to 2019. In these topmost productive journals, 11 journals each are published from the United Kingdom and the United States of America, 15 journals are published from India and 10 journals are published from the Netherlands. Based on the publications the *RSC Advances* journal from United Kingdom published the highest publications i.e. 6,578 articles (6.609%) followed by *Research Journal Of Pharmaceutical Biological And Chemical Sciences* (India) published 4,192 (4.212%)

articles, *AIP Conference Proceedings* (Germany) published 3,698 articles (3.715%), *Asian Journal Of Chemistry* (India) contributed 2,860 (2.873%) papers, *Tetrahedron Letters* from Netherlands published 2,826 (2.839%) papers, *Spectrochimica Acta Part A Molecular And Biomolecular Spectroscopy* (Netherlands) published 2,701 (2.714%) articles, *Journal Of Applied Polymer Science* (United States) published 2,563 (2.575%) articles, *International Journal Of Pharmacy And Pharmaceutical Sciences* (India) published 2,556 (2.568%) articles, *Journal Of Alloys And Compounds* (Netherlands) published 2,551 (2.563%), *Journal Of Materials Science Materials In Electronics* (New York) published 2,495 (2.507%) articles, *Journal Of The Indian Chemical Society* (India) published 2,232 (2.243%) papers, *Materials Today Proceedings* (UK) published 2,188 (2.198%) papers, *Chemistry select* (UK) published 2,136 (2.146%) papers and *Current Science* (India) published 2,072 (2.082%) papers.

Table 5: Source wise distribution of Indian contributions in Chemical Science literature

SN	Source Title	TP	%	Country
1	RSC Advances	6578	6.609	(United Kingdom)
2	Research Journal of Pharmaceutical Biological and Chemical Sciences	4192	4.212	India
3	AIP Conference Proceedings	3698	3.715	Germany
4	Asian Journal of Chemistry	2860	2.873	India
5	Tetrahedron Letters	2826	2.839	Netherlands
6	Spectrochimica Acta Part A Molecular and Biomolecular Spectroscopy	2701	2.714	Netherlands
7	Journal of Applied Polymer Science	2563	2.575	United States
8	International Journal of Pharmacy and Pharmaceutical Sciences	2556	2.568	India
9	Journal of Alloys And Compounds	2551	2.563	Netherlands
10	Journal of Materials Science Materials In Electronics	2495	2.507	New York
11	Journal of The Indian Chemical Society	2232	2.243	India
12	Materials Today Proceedings	2188	2.198	United Kingdom
13	Chemistry select	2136	2.146	United Kingdom
14	Current Science	2072	2.082	India
15	Journal of Physical Chemistry B	2054	2.064	United States
16	New Journal of Chemistry	2028	2.038	United Kingdom
17	Journal of Physical Chemistry C	2018	2.028	United States
18	International Journal of Biological Macromolecules	2008	2.017	Netherlands
19	Journal of Molecular Structure	1973	1.982	United Kingdom
20	Journal of Food Science and Technology	1831	1.840	India
21	Industrial and Engineering Chemistry Research	1828	1.837	United States
22	International Journal of Pharma and Bio Sciences	1819	1.828	India

23	Journal of Applied Physics	1811	1.820	United States
24	Journal of Molecular Liquids	1799	1.807	Netherlands
25	Materials Research Express	1770	1.778	United Kingdom
26	Applied Surface Science	1757	1.765	Netherlands
27	International Journal of Chemtech Research	1720	1.728	India
28	Physical Chemistry Chemical Physics	1709	1.717	Unites States
29	Acta Crystallographica Section E Structure Reports Online	1682	1.690	United Kingdom
30	Chemical Communications	1627	1.635	United Kingdom
31	Dalton Transactions	1597	1.605	United Kingdom
32	Journal of Chemical and Pharmaceutical Sciences	1576	1.583	India
33	Bioresource Technology	1569	1.576	Netherlands
34	Scientific Reports	1563	1.570	United Kingdom
35	Asian Journal of Pharmaceutical and Clinical Research	1551	1.558	India
36	Materials Chemistry and Physics	1550	1.557	Netherlands
37	Journal of Chemical Sciences	1519	1.526	India
38	Sensors and Actuators B Chemical	1504	1.511	Netherlands
39	PLOS One	1481	1.488	Unites States
40	Journal of Chemical Physics	1461	1.468	United States
41	Ceramics International	1443	1.450	United Kingdom
42	Inorganic Chemistry	1352	1.358	United States
43	Materials Letters	1331	1.337	Netherlands
44	Journal of Chemical and Pharmaceutical Research	1319	1.325	India
45	Chemical Physics Letters	1312	1.318	Netherlands
46	International Journal of Pharmaceutical Sciences Review and Research	1297	1.303	India
47	Medicinal Chemistry Research	1265	1.271	United States
48	Journal of Nanoscience and Nanotechnology	1263	1.269	United States
49	Research Journal of Pharmacy and Technology	1253	1.259	India
50	Bulletin of Materials Science	1243	1.249	India
		99531	100.00	

5.6. Language-wise distribution of publications of Indian Chemical Science research

Table 6 reveals the language-wise distribution of publications, the scientists' researchers from Indian chemical science literature are published in different languages; English, Chinese, Japanese, German, Welsh, French, Estonian and Danish. It is observed that the majority (99.909%) of articles published in English language, 64 (0.014 %) articles published in French language and very less number of articles are published in remaining languages.

Tabl 6: Language-wise distribution of publications of Indian Chemical Science research

SN	Language	TP	%
1	English	469515	99.909
2	French	64	0.014
3	Turkish	58	0.012
4	Spanish	57	0.012
5	German	40	0.009
6	Croatian	29	0.006

7	Portuguese	28	0.006
8	Russian	24	0.005
9	Bosnian	21	0.004
10	Polish	20	0.004
11	Chinese	19	0.004
12	Serbian	13	0.003
13	Japanese	9	0.002
14	Italian	6	0.001
15	Korean	6	0.001
16	Arabic	5	0.001
17	Lithuanian	3	0.001
18	Moldavian	3	0.001
19	Moldovan	3	0.001
20	Romanian	3	0.001
21	Slovenian	3	0.001
22	Malay	2	0.000
23	Czech	1	0.000
24	Estonian	1	0.000
25	Indonesian	1	0.000
26	Macedonian	1	0.000
27	Slovak	1	0.000
28	Ukrainian	1	0.000
29	Undefined	6	0.001
		469943	**100**

5.7. Channels used for Communicating Chemical Science Research

The channels used for communicating of Chemical Science research include articles published in the journals, reviews, conference and seminars proceedings, editorial materials, corrections and book chapters. This study has observed a total of 469689 publications inchemical science from India It has been observed from the table there are many communicating channels are used by scientists to publish their research articles in Indian chemical science literature. The majority of publications are published in Journals i.e. 402386 (85.%), followed by Conference Paper 249797 (8.27%) publications, Reviews 24236 (5.16%) are papers published, Book Chapter 14617 (0.18%) papers are published. and less than 1% of articles are published in other communication channels (table 7 & Fig 3).

Table 7: Channels used for Communicating Chemical Science Research

Sl.No	Document Type	TP	%
1	Article	402386	85.6
2	Conference Paper	24797	8.27
3	Review	24236	5.16
4	Book Chapter	14617	0.18
5	Book	850	0.18
6	Letter	618	0.13
7	Note	597	0.12
8	Short Survey	464	0.09
9	Editorial	422	0.08
10	Erratum	280	0.05

11	Data Paper	198	0.04
12	Retracted	116	0.02
13	Business Article	2	0
14	Undefined	106	0.02
	Total	**469689**	**100**

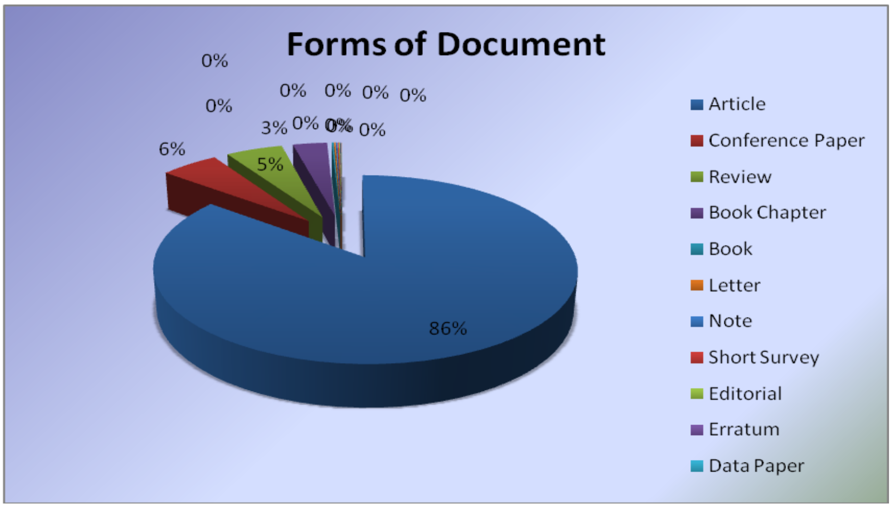

Fig. 3: Channels used for Communicating Chemical Science Research

5.8. Organizational / Institution productivity in the field of Chemical Science literature

Table 8 reveals the ranking list of the top 50 highly productive Research Institutions in India based on their highest publications, citations, average citations per publication and h-index. According to the Scopus database Indian Institute of Science, Bengaluru contributed the highest publications to the field of chemical science i.e. 15510 (3.537%) publications, followed by Bhabha Atomic Research Centre, Mumbai published 2.785 % i.e. 12142 Indian Institute of Technology Kharagpur Published 10263 (2.354%) papers next to Council of Scientific and Industrial Research India published 10232 (2.347%) of papers Indian Institute of Technology, Bombay published 8972 (2.058%) papers, Indian Institute of Technology Madras Published 8535 (1.957%) articles, University of Delhi Published 8151 (1.869%) published.

Table 8: Organizational / Institution productivity in the field of Chemical Science research

SN	Affiliation	TP	%
1	Indian Institute of Science, Bengaluru	15510	3.557
2	Bhabha Atomic Research Centre	12142	2.785
3	Indian Institute of Technology Kharagpur	10263	2.354

4	Council of Scientific and Industrial Research India	10232	2.347
5	Indian Institute of Technology, Bombay	8972	2.058
6	Indian Institute of Technology Madras	8535	1.957
7	University of Delhi	8151	1.869
8	National Chemical Laboratory India	7899	1.812
9	Banaras Hindu University	7845	1.799
10	Indian Institute of Technology Delhi	7600	1.743
11	Indian Institute of Chemical Technology	7550	1.732
12	Jadavpur University	7486	1.717
13	Indian Institute of Technology Kanpur	6941	1.592
14	Anna University	6504	1.492
15	Vellore Institute of Technology, Vellore	6398	1.467
16	Indian Association for the Cultivation of Science	6322	1.450
17	Indian Institute of Technology Roorkee	5808	1.332
18	University of Calcutta	5560	1.275
19	Panjab University	5502	1.262
20	Academy of Scientific and Innovative Research AcSIR	5237	1.201
21	Aligarh Muslim University	5018	1.151
22	Indian Institute of Technology Guwahati	4987	1.144
23	Institute of Chemical Technology	4971	1.140
24	Annamalai University	4750	1.089
25	University of Hyderabad	4264	0.978
26	University of Madras	3948	0.905
27	Savitribai Phule Pune University	3910	0.897
28	Tata Institute of Fundamental Research, Mumbai	3797	0.871
29	Bharathiar University	3705	0.850
30	Jawaharlal Nehru Centre for Advanced Scientific Research	3383	0.776
31	National Physical Laboratory India	3318	0.761
32	Indian Institute of Technology Banaras Hindu University	3090	0.709
33	SRM Institute of Science and Technology	3088	0.708
34	Sri Venkateswara University	3038	0.697
35	Birla Institute of Technology and Science, Pilani	3031	0.695
36	Guru Nanak Dev University	3007	0.690
37	ICAR - Indian Agricultural Research Institute, New Delhi	2988	0.685
38	Indira Gandhi Centre for Atomic Research	2978	0.683
39	Jawaharlal Nehru University	2966	0.680
40	Indian Institute of Chemical Biology	2907	0.667
41	SASTRA Deemed University	2881	0.661
42	University of Mysore	2823	0.647
43	Jamia Millia Islamia	2817	0.646
44	National Institute for Interdisciplinary Science and Technology	2773	0.636
45	Saha Institute of Nuclear Physics	2767	0.635
46	Shivaji University	2749	0.630
47	Indian Institute of Technology Indian School of Mines, Dhanbad	2670	0.612
48	Bharathidasan University	2664	0.611
49	Central Electrochemical Research Institute India	2644	0.606
50	King Saud University	2616	0.600
	Others	**175031**	**40.141**
	Total	**436036**	**100**

5.9. Most Productive Authors in the field of Chemical Science research

The most productive authors of Indian chemical science research are listed in table 5. It is worth to note that Hong, B. top in the list by contributing 1025 (2.184%) papers, followed by Tyurin, N. contributed 1011 (2.154%) 213 papers Dutta, D. Contributed 1010 (2.152%) papers, Velkovska, J. Contributed 996 (2.122%) papers, Martinez, G. Contributed 991 (2.111%) papers, Hohlmann, M. Contributed 952 (2.028%) papers, Das, S. Contributes 946 (2.015%) papers, Banerjee, S. Contributed 944 (2.011%) papers, Rose, A. Contributed 943 (2.009%) papers, Hofman, D.J. Contributed 940 (2.003%) papers, Betts, R.R. and Thomas, S. contributed 936 papers. The majority of the most productive authors belong to India (20), followed by 30 foreign authors who got placed in the top 50 list.

Table 9: Most productive authors in the field of Chemical Science research

SN	Author	TP	%
1	Hong, B.	1025	2.184
2	Tyurin, N.	1011	2.154
3	Dutta, D.	1010	2.152
4	Velkovska, J.	996	2.122
5	Martinez, G.	991	2.111
6	Hohlmann, M.	952	2.028
7	Das, S.	946	2.015
8	Banerjee, S.	944	2.011
9	Rose, A.	943	2.009
10	Hofman, D.J.	940	2.003
11	Betts, R.R.	936	1.994
12	Thomas, S.	936	1.994
13	Rakness, G.	934	1.990
14	Jung, H.	933	1.988
15	Mitselmakher, G.	933	1.988
16	Malgeri, L.	931	1.983
17	Mnich, J.	931	1.983
18	Onel, Y.	931	1.983
19	Pauss, F.	931	1.983
20	Rolandi, G.	931	1.983
21	Grab, C.	930	1.981
22	Moortgat, F.	930	1.981
23	Piccolo, D.	930	1.981
24	Blekman, F.	929	1.979
25	Denegri, D.	929	1.979
26	Ganjour, S.	929	1.979
27	Janot, P.	929	1.979
28	Mannelli, M.	929	1.979
29	Sphicas, P.	929	1.979
30	Sultanov, G.	929	1.979
31	Tully, C.	929	1.979
32	Wallny, R.	929	1.979
33	Yazgan, E.	929	1.979
34	Abbrescia, M.	928	1.977
35	Azzurri, P.	928	1.977
36	Bernet, C.	928	1.977
37	Dimitrov, A.	928	1.977
38	Dissertori, G.	928	1.977
39	Jarry, P.	928	1.977
40	Kaur, M.	928	1.977
41	Kim, G.N.	928	1.977
42	Klute, M.	928	1.977
43	Locci, E.	928	1.977

44	Maity, M.	928	1.977
45	Mans, J.	928	1.977
46	Pant, L.M.	928	1.977
47	Pape, L.	928	1.977
48	Pavlov, B.	928	1.977
49	Treille, D.	928	1.977
50	Aziz, T.	927	1.975
		46940	**100.000**

5.10. Highly Cited Papers in the field of Indian Chemical Science

Table – 10 shows characteristics of selected highly cited papers of India in chemical science. The list of such highly cited papers is presented based on the publication output of India in this area and 20 papers are identified as highly cited ones, who have received citations from 2963 to 6797 from 2000 to 2019. These 20 high cited papers were published in 19 journals including 2 papers in *Chinese Physics C*. Most of the papers are having multiple authors (Three or more authors), three papers are the double author and seventeen papers are having more than two authors. The top-cited paper was Titanium dioxide photocatalysis authored by Rao, Fujishima, A., Rao, T.N., Tryk, D.A. A. published in *Journal of Photochemistry and Photobiology C* in the year 2000 and this paper has received 6797 citations, followed by Review of particle physics, authored by Review of particle physics published Chinese Physics C in the year 2014, and this paper received 5942 citations, Appropriate body-mass index for Asian populations and its implications for policy and intervention strategies authored by Nishida, C., Barba, C., Cavalli-Sforza, T., (...), Yoshiike, N., Zimmet, P. published in The Lancet in the year 2004 and this paper received 5938 citations, Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC authored by Chatrchyan, S., Khachatryan, V., Sirunyan, A.M., (...), Swanson, J., Wenman, D. published in *Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics* in the year 2010 this paper received 5015 citations. Further, Reactive oxygen species and antioxidant machinery in abiotic stress tolerance in crop plants', authored by Gill, S.S., Tuteja, N. published in *Plant Physiology and Biochemistry* received 4823 citations, The CMS experiment at the CERN LHC', authored by Chatrchyan, S., Hmayakyan, G., Khachatryan, V., (...), Umaraliev, A., Yuldashev, B.S.. published in *Journal of Instrumentation* in the year 2008 paper received 4768 citations, 'The International Classification of Headache Disorders, 3rd edition (beta version)' authored by Olesen, J., Bes, A., Kunkel, R., (...), De Siqueira, S., Wöber-Bingöl, Published in *Cephalalgia* in the year 2013 this paper received 4488 citations. Planck 2015 results: XIII. Cosmological parameters authored by Ade, P.A.R., Aghanim, N., Arnaud, M., (...), Zacchei, A., Zonca, A.. published in *Astronomy and Astrophysics* in the year 2016 received 4464 citations, Review of particle physics authored by Eidelman, S., Hayes, K.G., Olive, K.A., (...), Zenin, O.V., Zhu, R.-Y. Published in *Chinese Physics* C in the year 2004, 4011 citations received, Tissue-based map of the human proteome authored by Uhlén, M., Fagerberg, L., Hallström, B.M., (...), Nielsen, J., Pontén, F. in the journal of Science, in the year of 2015 and 3817 citations, Silver nanoparticles as a new generation of antimicrobials authored by Rai, M., Yadav, A., Gade, A. in the journal of Biotechnology Advances, in this year of 2009 and received 3656 citations,

Table 10: Highly Cited Papers in the field of Indian Chemical Science

Title	Authors	Source Title	Year	Citation	Rank
Titanium dioxide photocatalysis	Fujishima, A., Rao, T.N., Tryk, D.A.	Journal of Photochemistry and Photobiology C: Photochemistry Reviews1(1), pp. 1-21	2000	6797	1
Review of particle physics	Olive, K.A., Agashe, K., Amsler, C., (...), Lugovsky, V.S., Schaffner, P.	Chinese Physics C 38(9),090001	2014	5942	2
Appropriate body-mass index for Asian populations and its implications for policy and intervention strategies	Nishida, C., Barba, C., Cavalli-Sforza, T., (...), Yoshiike, N., Zimmet, P.	The Lancet 363(9403), pp. 157-163	2004	5938	3
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6. Conclusion

The article suggests an update on the current status of Chemicals science research in India in the world context. This evaluation is based on the scientometric analysis of chemical science research publications by India and the world. The data was sourced from the Scopus database covering the last two-decade period 2000 – 2019. India is the 5th most productive country in the world of chemical science research. This paper describes the status of chemical science research at the global, national, institutional and individual research scientist level. The study is based on 20 years of Indian research data in the subject (covering 49,978 publications) sourced from the Scopus database during 2000-2019. The chemical science research registered absorbed that 20 years study period, a total of 469,689 publications are published. Out of 20 years, the year 2019 was most productive with 49,978 (10.64%) publications, followed by 46726 (9.94%) in the year 2018, 42592 (9.06%) in the year 2017 and the least number of 5556 (1.18%) publications in the year 2000. The compound annual growth rate is 8.325%. The highest number of papers published in the subject area is Chemistry 11, 65,377 publications followed by Materials Science 1, 19,949 research papers. The topmost productive journals 11 journals each are published from the United Kingdom and the United States of America, 15 journals are published from India and 10 journals are published from the Netherlands. To productive author is identified Hong, B. top in the list by contributing 1025 (2.184%) papers, followed by Tyurin, N. contributed 1011 (2.154%) 213 papers. This type of studies evaluate the research giving a direction for new areas to be explored. It also helps to compare with research globally and learn.

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RASĀYAN *J. Chem.*
Vol. 13 | No. 4 |2498-2507| October - December | 2020
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

HEAVY METAL CONTAMINATIONS AND HEALTH RISK ASSESSMENT FROM FRUITS AND VEGETABLES IN BANGALORE RURAL MARKETS, KARNATAKA, INDIA.

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ABSTRACT

The study is to assess heavy metals contamination in vegetables and fruits in Bangalore Rural taluk markets such as Nelamangala, Doddaballapura, Devanahalli and Hosakote. Samples randomly collected from these markets were analyzed for heavy metals, *viz*. Lead, Chromium, Cadmium, Arsenic, Mercury and Copper in vegetables like Tomato (Solanum lycopersicum), Brinjal (*Solanum melongena*), Radish (*Raphanus sativus*), Carrot (*Daucus carota*), Cauliflower (*Brassica oleracea*), Beans (*Phaseolus vulgaris*), Spinach (*Spinacea oleracea*), Banana (*Musa paradisiaca*), Mango (*Mangifera indica*) by using standard methods, such as ICP-MS. The Metal pollution index and Hazard quotient were calculated. The results indicate that the presence of heavy metals in vegetables and fruits was beyond the permissible limits of human consumption set by FAO/WHO. Consumption of contaminated fruits and vegetables may disturb biochemical and biological activities in human beings.

Keywords: Heavy Metals, Vegetables, Metal Pollution Index, Hazards Quotient and ICP-MS

INTRODUCTION

Though heavy metals are natural elements found in the earth's crust, the environmental pollution is due to anthropogenic activities, fertilizer and pesticide use in agricultural practices.[1] Vegetable is a part of the common diet throughout the world, as they provide essential nutrients, antioxidants and metabolites and act as a buffer for acid substances during the digestion process.[2] But with plants being good absorbers of metals from the soil, both essential and toxic elements were present in vegetables over a wide range of concentrations.[3] The intake of contaminated vegetables may lead to many lingering diseases. For instance, continuous exposure to Cd can cause pulmonary effects like emphysema, bronchiolitis, and alveolitis.[4] Industrial and agricultural drainage contains pesticides, fertilizers, effluents and runoff, in addition to sewage, which contaminates water bodies and deposits sediments with huge quantities of inorganic anions and heavy metals.[5] The main sources of metal pollution from human activities are industrial, petroleum contamination and sewage disposal. An organic pollutant can undergo decomposition but heavy metals remain in the environment for a long time and impact the human health. In this study, heavy metals such as Lead, Cadmium, Copper, Mercury, Arsenic and Chromium were analyzed in samples collected in different market places of Nelamangala, Doddaballapura, Devanahalli and Hosakote taluks of Bangalore rural district.[6] Intake of contaminated vegetables and fruits causes health risk.[7] This study provides data on the levels of heavy metals in vegetables and fruits found in Bangalore rural markets, which would be a baseline data for further studies.[8] The impact of metals present in vegetables and their hazards calculated. Since heavy metal contamination of food items is one of the most important aspects of food quality assurance, the present investigation focused on Metal Pollution Index (MPI), Average Daily Index (ADI), Hazard Quotient (HQ) and Hazard Index (HI) as an advanced part of the research work.[9]

Rasayan J. Chem., 13(4), 2498-2507(2020)
http://dx.doi.org/10.31788/ RJC.2020.1346039

Metal Pollution Index (MPI)

The overall load of metals in each vegetable growing at each site was assessed by the metal pollution index.[10] It is the geometric mean of the concentration of all metals in the sample.

$$\text{MPI (mg/kg)} = (C_1 \times C_2 \times C_3 \ldots\ldots C_n)^{1/n} \qquad (1)$$

Where C_n = Concentration of metal n in the sample.

Average Daily Index (ADI)

Average Daily Index is a parameter to calculate how much amount of heavy metal intake by a person per day (mg/person/day)

Mathematically it can be calculated by the given formula:

$$\text{ADI} = \text{Cm} \times \text{D intake x C Factor} \qquad (2)$$

Where,

Cm: Average heavy metal concentration of dry weight of the sample (mg/g)

D intake: Daily intake vegetable (g/day). WHO guidelines suggest an average daily consumption of vegetables of 300 to 350 g per person. The mean of 325 g/person/day was used in calculating the ADI values and the average weight of the person was taken as 60 kg.

C factor: The conversion factor of 0.085 was used to convert fresh vegetable weight to dry weight.

Hazard Quotient (HQ)

Hazard quotient can be used to screen the level of risk associated with the consumption of contaminated food (USEPA).[11] Hazard quotient is a proportion of the probable exposure to an element/chemical and level at which no negative impacts are expected. If $HQ < 1$, no potential health effects are expected from exposure, but if $HQ > 1$, there are potential health risks.[12] Hazard quotient for adults and children associated with the intake of metals along with vegetables was assessed using the formula:

$$\text{HQ} = \text{ADI}/(\text{RfD}) \qquad (3)$$

Where, ADI = Average daily intake of metal (mg/kg/day), RfD = Reference oral dose of metal (mg/kg of body weight/day).The oral reference dose for As, Cr, Cu, Pb, Cd and Hg reported was 0.0003, 0.3, 0.04, 0.004, 0.001, 0.0001 mg/kg/day.[13]

Hazard Index (HI)

Hazard Index (HI) was developed to evaluate the potential risk of more than one heavy metal to human health. HI is the sum of hazard quotients of all heavy metals, as mentioned in eq.4. It assumes that the magnitude of the adverse effect will be proportional to the sum of multiple metal exposures. It also assumes similar working mechanisms that linearly affect the target organ.

$$\text{Hazard Index (HI)} = \Sigma\,\text{HQ} = \text{HQAs} + \text{HQCr} + \text{HQCu} + \text{HQPb} + \text{HQCd} + \text{HQHg} \qquad (4)$$

If the $HI > 1$, there is a concern for potential health effects.[14] Though there was no apparent risk when each metal was analyzed individually, the risk could be higher when all metals are considered.

EXPERIMENTAL

Study Area

Bangalore rural district covers Nelamangala, Doddaballapura, Devanahalli and Hosakote taluks which are located at 12°15’ and 13°35’ North latitude 77°05’ and 78°0’ East and Longitude spread over 2259 sq. km. The average annual rainfall is about 859.6 mm and temperature ranges between 15°C and 34°C. Due to proximity to Bangalore city, there are a lot of industrial developments in this area.[15]

Sampling Designs and Analysis

Vegetable and fruit samples were collected for this study at different locations of Doddaballapura, Nelamangala, Devanahalli and Hosakote taluks separately in clean plastic zip-lock covers, labeled and brought to Laboratory for preparation. The samples were rinsed with double distilled water to remove dust, pollutants and fertilizers. Vegetable samples were cut into small pieces, air-dried for 2 days and dried at 100±1°C in a hot air oven for 3 hours.[16] Samples were then grounded in warm condition, passed through a sieve and then uniformly mixed. Composite samples were analyzed for Arsenic, Chromium, Copper, Lead, Cadmium and Mercury were carried out by standard methods, such as ICPMS (FSSAI Manual 2016 - Method 3).

Fig.-1: Bangalore Rural District and Its Taluks

Quality Control Analysis

Prepared NIST grade heavy metal standard solution (1000 mg/L) namely. Arsenic, Chromium, Copper, Lead, Cadmium and Mercury. The standard curve plotted using various concentrations against sample solution and analyzed for metal content. In vegetable samples analyzed by using FSSAI Manual 2016 (Method 3).

RESULTS AND DISCUSSION

The results of heavy metals concentration and impact analysis parameters such as MPI, ADI, HQ and HI are summarized in Tables-1 to 13 and compared against corresponding established permissible limits. The Heavy Metals Standard legal limits reported for Pb, Cr, Cd, As, Hg and Cu in the vegetables were 0.2, 2.3, 0.1,0.1, 0.03 and 40 (mg/kg) respectively.[17]

Table-1: Heavy Metal Concentration of Vegetable in Nelamangala.

Metals/ Vegetables	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	0.380	0.103	BDL	0.083	0.052	BDL	0.072	BDL	0.032
Cr	6.203	3.034	4.148	3.634	4.143	1.543	4.813	0.913	0.153
Cu	13.937	2.133	2.501	2.133	3.259	0.059	3.909	9.259	15.609
Pb	1.780	1.202	1.124	0.702	2.502	0.042	1.801	0.502	29.201
Cd	0.208	0.061	BDL	0.052	0.060	0.1560	0.020	0.810	0.050
Hg	BDL	0.030	0.011	0.050	0.013	0.021	0.041	BDL	0.011

Table-2: Acceptable Daily Intake (ADI) of Vegetables in Nelamangala

Metals/DIR	Tomato	Brinjal	Radish	Carrot	Cauliflower	Beans	Spinach	Banana	Mango
As	0.1050	0.0285	BDL	0.0229	0.0144	BDL	0.0199	BDL	0.0088
Cr	1.7136	0.8381	1.1459	1.0039	1.1445	0.4263	1.3296	0.2522	0.0423
Cu	3.8501	0.5892	0.6909	0.5892	0.9003	0.0163	1.0799	2.5578	4.3120
Pb	0.4917	0.3321	0.3105	0.1939	0.6912	0.0116	0.4975	0.1387	8.0668
Cd	0.0575	0.0169	BDL	0.0144	0.0166	0.0431	0.0055	0.2238	0.0138
Hg	BDL	0.0083	0.0030	0.0138	0.0036	0.0058	0.0113	BDL	0.0030

Heavy metals concentration in nine vegetable and fruit samples consumed by all classes of Indian citizens were analyzed and results are summarised in Tables-1 to 13. The safe limit reported in vegetables for Arsenic, Chromium, Copper, Lead, Cadmium and Mercury are 0.1, 2.3, 40.0, 0.2, 0.1 and 0.03 mg/kg respectively.[18]The arsenic concentration is higher than the safe limit in tomato and brinjal, but the other values are found to be within the safe limit in the vegetables at Nelamangala as shown in Table-1.

Table-3: HQ and HI Values of vegetables in Nelamangala.

Metals/DIR	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	5.83	1.58	BDL	1.27	0.80	BDL	1.11	BDL	0.49
Cr	0.10	0.05	0.06	0.06	0.06	0.02	0.07	0.01	0.00
Cu	1.60	0.25	0.29	0.25	0.38	0.01	0.45	1.07	1.80
Pb	2.05	1.38	1.29	0.81	2.88	0.05	2.07	0.58	33.61
Cd	0.96	0.28	BDL	0.24	0.28	0.72	0.09	3.73	0.23
Hg	BDL	1.38	0.51	2.30	0.60	0.97	1.89	BDL	0.51
Hazard Index(HI)	10.54	4.92	2.15	4.92	4.99	1.76	5.68	5.39	36.64

Table 4: Heavy Metal Concentration in Vegetables in Devanahalli

Metals/ vegetables	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	0.250	0.035	BDL	BDL	0.091	0.052	0.150	BDL	0.060
Cr	4.613	3.113	2.253	0.063	3.213	1.153	3.113	0.083	0.251
Cu	15.509	18.159	15.209	12.301	5.559	0.159	2.501	8.209	15.209
Pb	1.122	1.902	3.501	4.202	6.502	0.091	4.222	0.801	31.202
Cd	0.152	0.012	0.040	0.062	3.212	BDL	3.152	0.081	6.102
Hg	0.112	0.021	0.014	0.042	0.112	0.024	BDL	0.011	0.082

Table-5: Acceptable Daily Intake (ADI) Vegetables in Devanahalli.

Metals/ DIR	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	0.0691	0.0097	BDL	BDL	0.0251	0.0144	0.0414	BDL	0.0166
Cr	1.2743	0.8600	0.6224	0.0174	0.8876	0.3185	0.8600	0.0229	0.0693
Cu	4.2844	5.0164	4.2015	3.3982	1.5357	0.0439	0.6909	2.2677	4.2015
Pb	0.3100	0.5254	0.9672	1.1608	1.7962	0.0251	1.1663	0.2213	8.6196
Cd	0.0420	0.0033	0.0111	0.0171	0.8873	BDL	0.8707	0.0224	1.6857
Hg	0.0309	0.0058	0.0039	0.0116	0.0309	0.0066	BDL	0.0030	0.0227

Table-6: HQ and HI Values of Vegetables in Devanahalli

Metals/ vegetables	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	3.84	0.54	BDL	BDL	1.40	0.80	2.30	BDL	0.92
Cr	0.07	0.05	0.03	0.00	0.05	0.02	0.05	0.00	0.00
Cu	1.79	2.09	1.75	1.42	0.64	0.02	0.29	0.94	1.75
Pb	1.29	2.19	4.03	4.84	7.48	0.10	4.86	0.92	35.91
Cd	0.70	0.06	0.18	0.29	14.79	BDL	14.51	0.37	28.09
Hg	5.16	0.97	0.64	1.93	5.16	1.11	BDL	0.51	3.78
Hazard Index(HI)	12.84	5.89	6.64	8.47	29.52	2.04	22.01	2.75	70.46

Table-7: Heavy Metal Concentration of Vegetables in Doddaballapura.

Parameter	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	0.120	0.292	BDL	BDL	0.020	BDL	0.710	0.022	BDL
Cr	4.113	1.213	4.051	9.213	8.113	0.711	2.213	0.081	0.090
Cu	10.209	18.509	6.501	3.109	6.509	5.201	6.909	9.201	11.210

Pb	1.512	8.201	3.622	2.812	7.301	0.150	5.212	2.550	42.202
Cd	0.080	0.020	0.152	0.035	0.040	0.020	0.090	0.901	8.020
Hg	0.025	3.314	2.102	1.019	0.195	BDL	0.080	BDL	0.142

The content of metals, *i.e.,* Cr, Zn, Cd and Cu in the tomato of the studied area was comparable with values reported in the city of Varanasi, India.[19] Chromium concentration is found to be more than the safe limit in all vegetables and fruits, except in beans.

Even though Chromium is essential for human beings and animals for lipid and carbohydrate metabolism up to 200µg/day, breaching normal concentration levels leads to hepatitis, gastritis, ulcers and lung cancer.[10] Copper is an essential micronutrient that functions as a biocatalyst, required for body pigmentation Copper concentration in all and vegetable were found to be within the safe limit. Lead concentration is higher than the safe limit in all vegetables and fruits, except beans. Accumulation of lead is mainly due to a large number of small scale industries, vehicular emissions, suspended road dust and diesel generator sets. Uptake of lead in plants is regulated by pH, particle size and Cat-ion exchange capacity of soil as well as by root exudation and another Physico-chemical parameters.[20]Cadmium is a highly toxic, non-essential, heavy metal that has no role in the biological process of living organisms. Even at a lower concentration of Cd in the food chain could be harmful. Cadmium concentration was found to exceed the safe limit in Tomato, Beans and Banana. Usage of contaminated water for irrigation, fertilizers, sewage and compost can rapidly increase the Cd uptake into plant tissues.[21] Mercury concentration exceeded the safe limit in brinjal, carrot and spinach. Mercury is found alarmingly higher concentrations in both tomato and cabbage samples. The Cu, Cd and Pb contents observed in the Spinacea leaves of the studied area were comparable with the values reported in the leaves found in Bangalore, Delhi and Bangladesh regions.[22]

Table-8: Acceptable Daily Intake (ADI) of Vegetables in Doddaballapura.

Metals/DIR	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	0.0332	0.0807	BDL	BDL	0.0055	BDL	0.1961	0.0061	-
Cr	1.1362	0.3351	1.1191	2.5451	2.2412	0.1964	0.6113	0.0224	0.0249
Cu	2.8202	5.1131	1.7959	0.8589	1.7981	1.4368	1.9086	2.5418	3.0968
Pb	0.4177	2.2655	1.0006	0.7768	2.0169	0.0414	1.4398	0.7044	11.6583
Cd	0.0221	0.0055	0.0420	0.0097	0.0111	0.0055	0.0249	0.2489	2.2155
Hg	0.0069	0.9155	0.5807	0.2815	0.0539	BDL	0.0221	BDL	0.0392

Table-9: HQ and HI Values of Vegetables in Doddaballapura

Metals/DIR	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	1.84	4.48	BDL	BDL	0.31	BDL	10.90	0.34	-
Cr	0.06	0.02	0.06	0.14	0.12	0.01	0.03	0.00	0.00
Cu	1.18	2.13	0.75	0.36	0.75	0.60	0.80	1.06	1.29
Pb	1.74	9.44	4.17	3.24	8.40	0.17	6.00	2.94	48.58
Cd	0.37	0.09	0.70	0.16	0.18	0.09	0.41	4.15	36.93
Hg	1.15	152.58	96.78	46.92	8.98	BDL	3.68	BDL	6.54
Hazard Index	6.34	168.74	102.46	50.81	18.75	0.87	21.82	8.48	93.33

From Table-4, in Devanahalli, it can be seen that Arsenic concentration exceeded the safe limit in Tomato and Spinach. Chromium concentration exceeded the safe limit in Tomato, Brinjal, Cauliflower, and Spinach, except in, Radish, Carrot, beans and Banana. Copper concentration in all the fruits and vegetable were within the safe limit. Lead concentration exceeded the safe limit in all vegetables and fruits except beans. Cadmium concentration exceeded the safe limit in Tomato, Cauliflower, Spinach and Mango. Mercury concentration exceeded the safe limit in Tomato, Carrot, Cauliflower and Mango. From Table-7, in Doddaballapura, it can be seen that Arsenic concentration was more than the safe limit in Tomato, Brinjal and Spinach. Chromium concentration exceeded the safe limit in Tomato, Radish, Carrot, Cauliflower and Spinach. Copper concentration in all fruits and vegetables sampled were within a safe limit. Lead concentration exceeded the safe limit in all vegetables and fruits, except beans. Cadmium concentration exceeded the safe limit in Radish, Banana and Mango. Mercury concentration exceeded the safe limit in Brinjal, Radish, Carrot, Cauliflower, Spinach and Mango.[23] From Table-10, in Hosakote, it can be seen that Arsenic concentration was higher than the safe limit in Spinach. Chromium concentration exceeded the safe limit in Tomato, Radish, Carrot, Cauliflower, Spinach and in others, was in the safe limit. Copper concentration in all the fruits and vegetables was within a safe limit. Lead concentration was higher than the safe limit in all vegetables and fruits, except Beans. Cadmium concentration was exceeded the safe limit in Tomato, Brinjal, Cauliflower, Beans, Spinach and Mango. Mercury concentration exceeded the safe limit in Brinjal, Cauliflower and others were in the safe limit. The impacts of heavy metal contamination on vegetables and fruits were analyzed by using HQ and HI.[24]

Table-10: Heavy Metal Concentration of Vegetables in Hosakote

Metals/ DIR	Tomato	Brinjal	Radish	Carrot	Cauli Flower	Beans	Spinach	Banana	Mango
As	0.032	0.041	0.080	0.060	0.052	BDL	0.580	0.030	BDL
Cr	2.513	1.916	4.210	3.183	5.215	0.150	3.213	0.050	0.901
Cu	3.521	13.521	9.519	5.809	14.501	3.519	3.219	10.529	13.419
Pb	2.201	5.925	6.502	3.901	7.525	0.082	9.701	7.582	25.501
Cd	0.900	0.622	0.021	0.092	1.902	0.291	0.212	0.041	9.512
Hg	BDL	0.032	0.012	0.011	0.132	BDL	0.011	BDL	0.081

Table 11: Acceptable Daily Intake (ADI) of Vegetables in Hosakote

Metals/DIR	Tomato	Brinjal	Radish	Carrot	Cauli flower	Beans	Spinach	Banana	Mango
As	0.0088	0.0113	0.0221	0.0166	0.0144	BDL	0.1602	0.0083	BDL
Cr	0.6942	0.5293	1.1630	0.8793	1.4406	0.0414	0.8876	0.0138	0.2489
Cu	0.9727	3.7352	2.6296	1.6047	4.0059	0.9721	0.8892	2.9086	3.7070
Pb	0.6080	1.6368	1.7962	1.0777	2.0788	0.0227	2.6799	2.0945	7.0447
Cd	0.2486	0.1718	0.0058	0.0254	0.5254	0.0804	0.0586	0.0113	2.6277
Hg	BDL	0.0088	0.0033	0.0030	0.0365	BDL	0.0030	BDL	0.0224

Table-12: HQ and HI Values of Vegetables in Hosakote.

Metals/ DIR	Tomato	Brinjal	Radish	Carrot	Cauli flower	Beans	Spinach	Banana	Mango
As	0.49	0.63	1.23	0.92	0.80	BDL	8.90	0.46	BDL
Cr	0.04	0.03	0.06	0.05	0.08	0.00	0.05	0.00	0.01
Cu	0.41	1.56	1.10	0.67	1.67	0.41	0.37	1.21	1.54
Pb	2.53	6.82	7.48	4.49	8.66	0.09	11.17	8.73	29.35
Cd	4.14	2.86	0.10	0.42	8.76	1.34	0.98	0.19	43.79
Hg	BDL	1.47	0.55	0.51	6.08	BDL	0.51	BDL	3.73
Hazard Index	7.61	13.37	10.52	7.06	26.04	1.84	21.97	10.59	78.44

Table-13: Metal Pollution Index (MPI) for Vegetables in Bangalore Rural

Site/Vegetables	Tomato	Brinjal	Radish	Carrot	Cauli flower	Beans	Spinach	Banana	Mango
Nelamangala	1.65	0.34	0.6	0.32	0.33	0.17	0.35	1.36	0.33
Devanahalli	0.84	0.31	0.58	0.39	1.25	0.12	1.73	0.22	1.24
Doddaballapura	0.5	1.24	1.98	1.23	0.63	0.32	0.86	0.52	2.17
Hosakote	0.89	0.71	0.42	0.4	1.4	0.34	0.72	0.35	2.99

Graphical representation of Metal pollution index for Vegetables and fruits are as follows:

Hazard Quotient (HQ)

The HQ values of all heavy metal were compared in all the vegetables and fruits. If the observed value of HQ >1, causes more potential health effects.[11, 15]

In Nelamangala Table-3, HQ value is higher than the safe limit for Arsenic in Tomato (5.83)>Brinjal (1.58) > Carrot (1.27) for Copper in Mango (1.80)>Tomato (1.60), for Lead in Mango (33.61) > Cauliflower (2.88) >Spinach (2.07) >Tomato (2.05) > Brinjal (1.38) > Raddish (1.29), for Cadmium in Banana (3.73), for Mercury in Carrot (2.30) > Spinach(1.89) > Brinjal(1.38) .
In Devanahalli Table-6, HQ value is higher for Arsenic in Tomato (3.84) > Spinach (2.30) > Cauliflower (1.40), for Copper in Brinjal (2.09) > Tomato (1.79) > Mango and Raddish (1.75) > Carrot (1.42), for Lead in Mango (35.91) > Cauliflower (7.48) > spinach (4.86) > Carrot(4.84) > Raddish(4.03) > Brinjal(2.19) > Tomato (1.29), for Cadmium in Mango (28.09) > Cauliflower (14.79), for Mercury in Tomato and Cauliflower (5.16) > Mango (3.78) > Carrot (1.93).

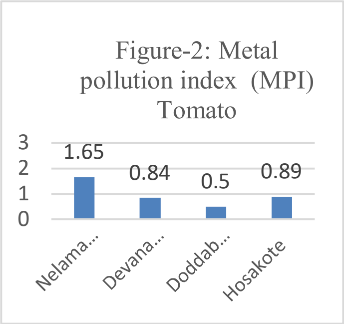
Figure-2: Metal pollution index (MPI) Tomato

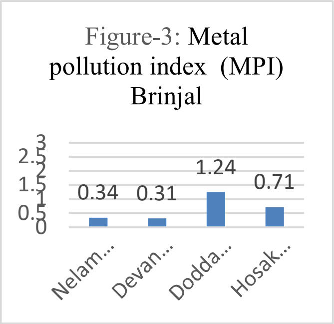
Figure-3: Metal pollution index (MPI) Brinjal

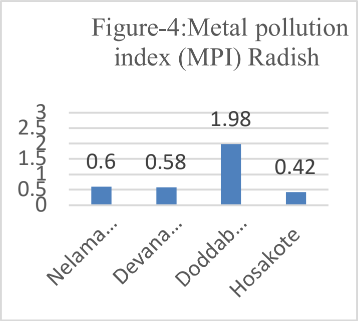
Figure-4:Metal pollution index (MPI) Radish

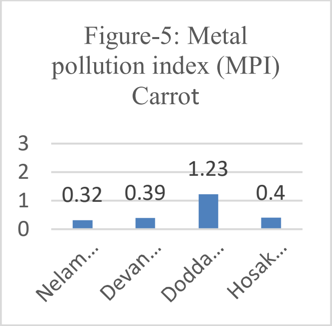
Figure-5: Metal pollution index (MPI) Carrot

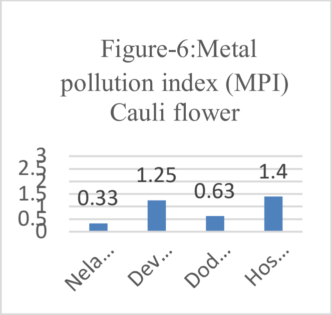
Figure-6:Metal pollution index (MPI) Cauli flower

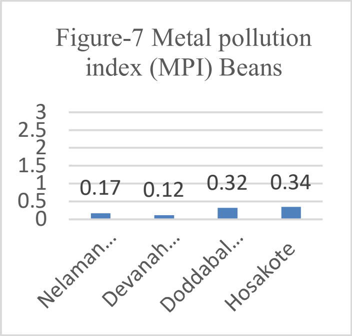
Figure-7 Metal pollution index (MPI) Beans

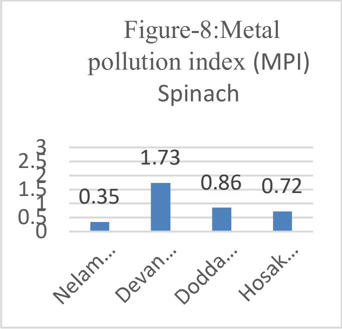
Figure-8:Metal pollution index (MPI) Spinach

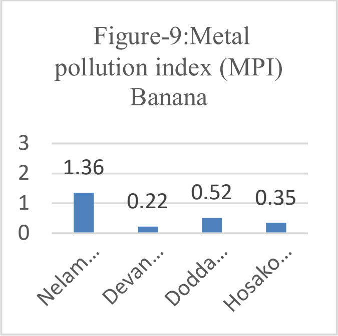
Figure-9:Metal pollution index (MPI) Banana

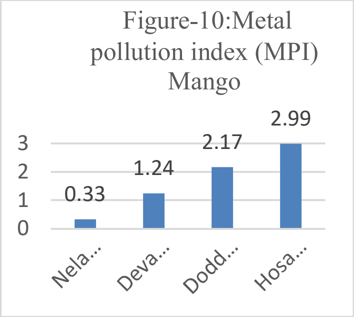
Figure-10:Metal pollution index (MPI) Mango

In Doddaballapura Table-9, HQ value is higher than the safe limit for Arsenic in Arsenic (10.90) > Brinjal (4.48) > Tomato (1.18) ,for Copper in Brinjal (2.13) > Banana (1.06) > Tomato (1.18), for Lead in Mango (48.58) > Brinjal (9.44) > Cauliflower (8.40) > spinach (6.00) > Raddish (4.17) > Carrot (3.24) > Tomato (1.74), for Cadmium in Mango (36.93), Banana (4.15), for Mercury in Brinjal (152.58), Raddish(96.78) > Carrot (46.92) > Cauliflower (8.98) ,Mango (6.54) ,Spinach (3.68) > Brinjal (1.38) and Tomato(1.15).

In Hosakote Table-12, HQ value is higher than the safe limit for Arsenic in Spinach (8.90) > Raddish (1.23) > Carrot (1.27), for Copper in Mango (1.54) > Cauliflower (1.67), Brinjal (1.56), Raddish (1.10), for Lead in Mango (29.35) > Spinach (11.17) > Banana (8.73) > Cauliflower (8.66) > Raddish (7.48) > Brinjal (6.82) > Tomato(2.53), for Cadmium in Mango (43.79) > Cauliflower (8.76) > Banana (3.73) > Brinjal (1.47), Mercury in Cauliflower(6.08) > Mango (3.73) > Brinjal (1.47).

Similar results were observed in Spinach for heavy metals (HQ>500) As, Mn, Cu, Cd, Pb and Hg content[24].

It shows from the HQ value that, most of the vegetables and fruits are higher than the safe in Bangalore Rural.

Hazard Index (HI)

The results from the Table-3, Nelamangala Market showed that the highest HI value found in Mango (36.64) > Tomato (10.54) > Spinach (5.68) > Banana (5.39) > Cauliflower (4.99) > Carrot (4.92) = Brinjal (4.92) > Radish (2.15) > Beans (1.76).

From the Table-6, it is observed that, HI exceeds the in Devanahalli market, Mango (70.46) > Cauliflower (29.52) > Spinach (22.01) > Tomato (12.84) > Carrot (8.47) > Radish (6.64) > Brinjal5.89) > Banana (2.75) > Beans (2.04).

The results from the Table-9, Doddaballapura Market, shows that, highest HI value found in Brinjal (168.7) > Radish (102.5) > Mango (93.3) > Carrot (50.81) > Spinach (21.81) > Cauliflower (18.8) > Banana (8.48) > Tomato (6.3) > Beans (0.87).

The results from the Table-12, Hosakote Market, shows that, highest HI value found in Mango (78.4) > Cauliflower (26.04) > Spinach (21.97) > Brinjal (13.37) > Banana (10.59) > Radish10.52) > Tomato (7.61) > Carrot (7.06) > Beans (1.84).

If the HI values exceeds 1.0, there is a concern for potential health effects.[25] From the observed values, the maximum health effects is found in Mango and less in Beans.

Metal Pollution Index (MPI)

The MPI for lead, chromium, cadmium, arsenic, mercury and copper for vegetables and fruits is found to be several folds higher MPI (> 1.0) as shown in Table-13. MPI values higher for Tomato (1.65), Banana (1.36) in Nelamangala, Cauliflower (1.25) and Mango (1.24) in Devanahalli, Mango (2.17), Raddish (1.98) and Brinjal (1.24) in Doddaballapura, Radish (2.99) in Hosakote.[26] If the MPI values exceed 1.0, there is a concern for potential health effects.

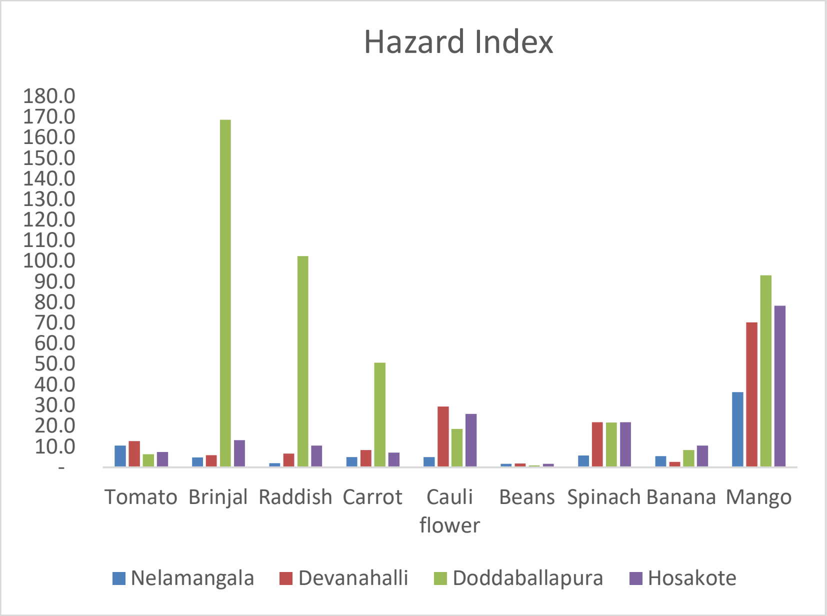

Fig.-11: Graphical Presentation of Hazard Index of Vegetables and Fruits

CONCLUSION

Experimental results for both vegetables and fruits were from the Average daily intake (ADI), Hazard Quotient (HQ), Hazard Index (HI) and Metal pollution index (MPI) showed that, consumption of vegetables and fruits may cause carcinogenic health risks to humans, due to high concentration of heavy metals such as Arsenic, Chromium, Copper, Lead, Cadmium and Mercury. After investigations, because of the health risk to the people of Bangalore Rural District., we recommend that awareness be created by Administrative Authorities and Public Health Department.

ACKNOWLEDGEMENT

The authors greatly acknowledge Vision group on Science and Technology (VGST), Government of Karnataka for providing K-FIST (L_1) grants to the PG Department of Chemistry and UGC for UGC-CPE / MRP grants to Government Science College (Autonomous), Bengaluru.

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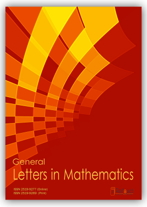
[RJC-6039/2020]

Available online at www.refaad.com
Gen.Lett. Math., 9(1) (2020), 9-16
Research Article

General Letters in Mathematics (GLM)
Journal Homepage: http://www.refaad.com/views/GLM/home.aspx
ISSN: 2519-9277 (Online) 2519-9269 (Print)



QSPR Analysis of Chemical Graph Theory

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Abstract

In this paper, we find the values of four important degree-based topological indices of molecular graph of alkane isomers. Further, we show that these parameters are highly correlated with physical properties of alkane isomers. . ©2019 All rights reserved.

Keywords: Alkane isomers,, Degree-based topological indices.
2010 MSC: 05C10, 57M15, 57M25.

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1. Introduction

Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \epsilon V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [4].

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. Hence chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. It has found to be a useful tool in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) [8, 5, 14]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices. In 1975, Randic [10] proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [4, 2, 11]. This theory had an important effect on the development of the chemical sciences.

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doi:10.31559/glm2020.9.1.2

Received 6 Jul 2018 : Accepted 12 Aug 2020

2. Computing Some New Degree-Based Topological Indices

We consider the following most studied degree based topological indices for QSPR study [12, 14, 15, 16].

Definition 2.1. Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u, then Arithmetic-Geometric Index $(AG_1 index)$ of G is defined as

$$AG_1(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

Where, $(AG_1 index)$ is considered for distinct vertices.
The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)\,(or\ d_G(v))$ denotes the degree of the vertex $u\,(or\ v)$.

Definition 2.2. The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u)+d_G(v)}{2}$, where $d_G(u)\ and\ d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.3. The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u).d_G(v)}{2}$, where $d_G(u)\ and\ d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.4. The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$, where $d_G(u)\ and\ d_G(v)$ are the degrees of the vertices u and v in G.

Motivation

By looking at the earlier results QSPR Analysis of Certain Degree-Based Topological Indices and QSPR Analysis of Degree-Based Topological Indices with physical properties of Benzenoid Hydrocarbons [7, 5, 6, 13].

3. Data Sources and Analytical Method

Energy of Alkane isomers are taken from [19, 7, 12, 5]. Seven physicochemical properties of Alkane isomers have been selected on the availability of a suitable body of data: *boiling point* (BP), *critical temperature* (CT), *critical pressure* (CP), *Molar volume* (CV), *Molar refraction* (MR), *Heat of Vaporization* (HV), *Surface tension* (ST). The values are compiled in Table 2.

4. Results and Discussion

In Table 3, the correlation coefficient of topological indices with physicochemical properties of alkane isomers are found to be good.

4.1. Regression Models

We have tested the following linear regression model

$$P = a + b(TI) \tag{4.1}$$

where, P=Physical property, TI=Topological Index. Using (4.1), we have obtained the following different linear models for each degree-based topological index, which are listed below.

Table 1: The topological indices (AG1 Index, SK Index, SK1 Index and SK2 Index) values of Alkane Isomers.

S.NO.	Compound Name	AG1 Index	SK Index	SK1 Index	SK2 Index
1	Butane	3.1213	5	4	8.5
2	2-methyl propane	3.46410	6	4.5	12
3	Pentane	4.123	7	6	12.5
4	2-methyl butane	4.3906	8	7	16.5
5	2,2 dimethyl propane	5	10	8	25
6	Hexane	5.1213	9	8	16.5
7	2-methyl pentane	5.2359	10	9	20.5
8	3- methyl pentane	5.3172	10	9.5	21
9	2,2-dimethyl butane	5.8713	12	11	30
10	2,3- dimethyl butane	5.6188	11	10.5	25
11	Heptanes	6.1213	11	10	20.5
12	2-methyl hexane	6.3906	12	11	24.5
13	3- methyl hexane	6.5767	12	11.5	25
14	3-ethylpentane	6.2438	12	12	25.5
15	2,2-dimethyl pentane	6.8713	14	13	34
16	2,3- dimethyl pentane	6.54530	13	13	29.5
17	2,4- dimethyl pentane	6.6600	13	12	28.5
18	3,3- dimethyl pentane	6.7426	14	14	35
19	Octane	7.1213	13	12	24.5
20	2-methylheptane	7.3906	14	13	28.5
21	3- methylheptane	7.3172	14	13.5	29
22	4- methylheptane	7.3172	14	13.5	29
23	3-ethylhexane	7.2438	14	14	29.5
24	2,2-dimethylhexane	7.8713	16	15	38
25	2,3- dimethylhexane	7.5453	15	15	33.5
26	2,4- dimethylhexane	7.5866	15	14.5	33
27	2,5- dimethylhexane	7.6600	15	14	32.5
28	3,3- dimethylhexane	7.7426	16	16	39
29	3,4- dimethylhexane	7.4719	15	15.5	34
30	3-ethyl-2-methylpentane	7.4719	15	15.5	34
31	3-ethyl-3-methylpentane	7.6139	16	17	40
32	2,2,3-trimethylpentane	7.9963	17	17.5	43.5
33	2,2,4- trimethylpentane	8.1406	17	16	42
34	2,3,3- trimethylpentane	7.9410	17	18	44
35	2,3,4- trimethylpentane	8.4401	16	16.5	38
36	Nonane	8.1213	15	14	28.5
37	2-methyloctane	8.3906	16	15	32.5
38	3-methyloctane	8.3172	16	15.5	33
39	4-methyloctane	8.3172	16	15.5	33
40	3-ethylheptane	8.2438	16	16	33.5
41	4- ethylheptane	8.2438	16	16	33.5
42	2,2-dimethylheptane	8.8713	18	17	42
43	2,3- dimethylheptane	8.5453	17	17	37.5
44	2,4- dimethylheptane	10.8960	17	16.5	37
45	2,5- dimethylheptane	8.5866	17	16.5	37
46	2,6- dimethylheptane	8.6600	17	16	36.5
47	3,3- dimethylheptane	8.7426	18	18	43
48	3,4- dimethylheptane	7.4719	17	17.5	38
49	3,5- dimethylheptane	8.5132	17	17	37.5
50	4,4- dimethylheptane	8.7426	18	18	43
51	3-ethyl-2-methylhexane	8.4719	17	17.5	38
52	4-ethyl-2-methylhexane	8.5132	17	17	37.5
53	3-ethyl-3-methylhexane	7.0229	18	19	44
54	2,2,4-trimethylhexane	9.0672	19	18.5	46.5
55	2,2,5- trimethylhexane	9.1406	19	18	46
56	2,3,3- trimethylhexane	8.9410	19	20	48
57	2,3,4- trimethylhexane	8.7000	18	19	42.6
58	2,3,5- trimethylhexane	8.8147	18	18	41.5
59	3,3,4- trimethylhexane	8.8676	19	20.5	48.5
60	3,3-diethylpentane	8.4852	18	20	40.5
61	2,2-dimethyl-3-ethylpentane	8.9229	19	20	44.75
62	2,3-dimethyl-3ethylpentane	8.8124	19	21	49
63	2,4-dimethyl-3-ethylpentane	8.7000	18	19	42.5
64	2,2,3,3-tetramethylpentane	9.3713	21	23	58.5
65	2,2,3,4- tetramethylpentane	9.2244	20	21	52
66	2,2,4,4- tetramethylpentane	9.6213	21	20	55.5
67	2,3,3,4- tetramethylpentane	9.1395	20	22	53

1. $AG_1\ Index\,(AG_1\,(G))$

$$Bp = 3.992 + 0.033AG_1\,(G) \tag{4.2}$$

$$CT = -0.976 + 0.03AG_1\,(G) \tag{4.3}$$

$$CP = 18.622 - 0.414AG_1\,(G) \tag{4.4}$$

$$MV = -3.525 + 0.069AG_1\,(G) \tag{4.5}$$

$$ST = -2.608 + 0.495AG_1\,(G) \tag{4.6}$$

Table 2: The physical and chemical properties (BP, MV, MR, HV, CT, CP, ST) of Alkane Isomers.

S.NO.	Compound Name	Bp(0C)	mv(cm3)	mr(cm3)	hv(kJ)	ct(0C)	cp(atm)	St(dyne/cm)
1	Butane	-0.500		20.68	22.44	152.01	37.47	12.46
2	2-methyl propane	-11.730		20.85	21.6	134.98	36	14.1
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00
5	2,2 dimethyl propane	9.503	112.074	25.7243	21.78	160.60	31.57	12.05
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42
7	2-methyl pentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38
8	3- methyl pentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12
9	2,2-dimethyl butane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30
10	2,3- dimethyl butane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26
12	2-methyl hexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29
13	3- methyl hexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44
15	2,2-dimethyl pentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02
16	2,3- dimethyl pentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96
17	2,4- dimethyl pentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15
18	3,3- dimethyl pentane	86.064	144.530	34.3323	33.02	263.00	30	19.59
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60
21	3- methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17
22	4- methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60
25	2,3- dimethylhexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99
26	2,4- dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05
27	2,5- dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73
28	3,3- dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63
29	3,4- dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67
33	2,2,4- trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77
34	2,3,3- trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56
35	2,3,4- trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81
41	4- ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80
43	2,3- dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34
44	2,4- dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30
45	2,5- dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30
46	2,6- dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83
47	3,3- dimethylheptane	137.00	176.897	43.6870	42.66	314.00	24.19	22.01
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22
54	2,2,4-trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31

Table 3: Correlation of topological indices with physicochemical properties of Alkane isomers.

	$Bp\left(^{0}\right)$	$ct\left(^{0}C\right)$	$cp\left(atm\right)$	$mv\left(cm^{3}\right)$	$st\left(\frac{dyne}{cm}\right)$	$hv\left(kJ\right)$	$mr\left(cm^{3}\right)$
AG_1	0.8463	0.8946	-0.8514	0.9186	0.8308	0.8614	0.9467
SK	0.8211	0.8945	-0.7661	0.8736	0.8097	0.8176	0.927
SK_1	0.8112	0.8959	-0.6730	0.8047	0.8290	0.7910	0.8864
SK_2	0.6841	0.7784	-0.5897	0.8047	0.6870	0.6522	0.7987

$$HV = -0.7 + 0.216AG_1\,(G) \tag{4.7}$$

$$MR = -1.586 + 0.236AG_1\,(G) \tag{4.8}$$

2. SK Index

$$Bp = 7.116 + 0.074SK\,(G) \tag{4.9}$$

$$CT = -4.689 + 0.069SK\,(G) \tag{4.10}$$

$$CP = 38.327 - 0.867SK\,(G) \tag{4.11}$$

$$MV = -9.553 + 0.155SK\,(G) \tag{4.12}$$

$$ST = -7.885 + 1.122SK\,(G) \tag{4.13}$$

$$HV = -3.07 + 0.478SK\,(G) \tag{4.14}$$

$$MR = -5.664 + 0.538SK\,(G) \tag{4.15}$$

3. SK_1 Index

$$Bp = 5.565 + 0.087SK_1\,(G) \tag{4.16}$$

$$CT = -8.611 + 0.083SK_1\,(G) \tag{4.17}$$

$$CP = 39.199 - 0.905SK_1\,(G) \tag{4.18}$$

$$MV = -12.542 + 0.172SK_1\,(G) \tag{4.19}$$

$$ST = -13.031 + 1.365SK_1\,(G) \tag{4.20}$$

$$HV = -5.945 + 0.549SK_1\,(G) \tag{4.21}$$

$$MR = -8.648 + 0.611SK_1\,(G) \tag{4.22}$$

4. SK_2 Index

$$Bp = 15.014 + 0.182SK_2\,(G) \tag{4.23}$$

$$CT = -16.102 + 0.178SK_2\,(G) \tag{4.24}$$

$$CP = 87.24 - 1.965SK_2\,(G) \tag{4.25}$$

$$MV = -12.542 + 0.172SK_2\,(G) \tag{4.26}$$

$$ST = -22.813 + 2.802SK_2\,(G) \tag{4.27}$$

$$HV = -8.052 + 1.122SK_2\,(G) \tag{4.28}$$

$$MR = -18.07 + 1.364SK_2\,(G) \tag{4.29}$$

By inspection of the data in Table 4 to Table 7, it is possible to draw a number of conclusions for the given topological indices like invariants.

The QSPR study of $AG_1\,(G)$ index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 4, one can easily verify that $AG_1\,(G)$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $AG_1\,(G)$ index with physical properties of alkane isomers lies between -0.8514 to 0.9467.

Further, the correlation coefficient value of $AG_1\,(G)$ index is very high for the MR of alkane isomers with r =0.9467.Thus the QSPR study reveals that the $AG_1\,(G)$ index is an useful tool in predicting the

Table 4: Statistical parameters for the linear QSPR model for $AG_1(G)$.

Physical Properties	N	a	b	r
Boiling point	67	3.992	0.033	0.8463
Critical temperature	67	-0.976	0.03	0.8946
Critical pressure	67	18.622	-0.414	-0.8514
Molar volume	65	-3.525	0.069	0.9186
ST	67	-2.608	0.495	0.8308
HV	67	-0.7	0.216	0.8614
MR	67	-1.586	0.236	0.9467

Table 5: Statistical parameters for the linear QSPR model for $SK(G)$.

Physical Properties	N	a	b	r
Boiling point	67	7.116	0.074	0.8211
Critical temperature	67	-4.689	0.069	0.8945
Critical pressure	67	38.327	-0.867	-0.7661
Molar volume	65	-9.553	0.155	0.8736
ST	67	-7.885	1.122	0.8097
HV	67	-3.07	0.478	0.8176
MR	67	-5.664	0.538	0.927

Table 6: Statistical parameters for the linear QSPR model for $SK_1(G)$.

Physical Properties	N	a	b	r
Boiling point	67	5.565	0.087	0.8112
Critical temperature	67	-8.611	0.083	0.8959
Critical pressure	67	39.199	-0.905	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-13.031	1.365	0.829
HV	67	-5.945	0.549	0.791
MR	67	-8.648	0.611	0.8864

Table 7: Statistical parameters for the linear QSPR model for $SK_2(G)$.

Physical Properties	N	a	b	r
Boiling point	67	15.014	0.182	0.6841
Critical temperature	67	-16.102	0.178	0.7784
Critical pressure	67	87.24	-1.965	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-22.813	2.802	0.687
HV	67	-8.052	1.122	0.6522
MR	67	-18.07	1.364	0.7987

physical properties of alkane isomers. The QSPR study of $SK(G)\, index$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 5, one can easily verify that $SK(G)\, index$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK\left(G\right) index$ with physical properties of alkane isomers lies between -0.7661 to 0.927. Further, the correlation coefficient value of $SK\left(G\right) index$ index is very high for the MR of alkane isomers with r =0.927.Thus the QSPR study reveals that the $SK\left(G\right) index$ index is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of $SK_1\left(G\right) index$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 6, one can easily verify that $SK_1\left(G\right) index$ shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK_1\left(G\right) index$ with physical properties of alkane isomers lies between -0.673 to 0.8959. Further, the correlation coefficient value of $SK_1 index$ is very high for the CT of alkane isomers with r =0.8959.Thus the QSPR study reveals that the $SK_1\left(G\right) index$ is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of $SK_2\left(G\right) index$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 7, one can easily verify that $SK_2\left(G\right) index$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK_2\left(G\right) index$ with physical properties of alkane isomers lies between -0.673 to 0.7987. Further, the correlation coefficient value of $SK_2\left(G\right) index$ is very high for the MR of alkane isomers with r =0.7987.Thus the QSPR study reveals that the $SK_2\left(G\right) index$ is an useful tool in predicting the physical properties of alkane isomers.

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 07 (A), pp. 39115-39120, July, 2020

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

BIOACCUMULATION OF XENOBIOTICS FROM SEWAGE BY AQUATIC MACROPHYTE

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1107.5444

ARTICLE INFO

Article History:

Received 06th April, 2020
Received in revised form 14th May, 2020
Accepted 23rd June, 2020
Published online 28th July, 2020

Key Words:

Heavy metals, accumulation, sewage, toxicity, biochemical parameters.

ABSTRACT

Increasing urbanization, industrialization, and over population and anthropogenic activities have contributed huge quantities, industrial and domestic waste water, which contains huge quantities of xenobiotics that leads to undesirable changes of the environment.

The *xenobiotics* disrupts the food chain and some toxicants are lethal even a lower concentrations. The prevailing purification technologies used for the removal of contaminants from the sewage are not only costly but causes negative impact on ecosystem subsequently .The aquatic plants have the potentiality to accumulate xenobiotics, as they were tolerant and able to withstand the pollution stress. They serve as a tool for the remediation of xenobiotics from the aquatic ecosystem. Phytoremediation is an emerging "Green Bioengineering Technology" and this concept is cheaper and alternative that hardly cost civil engineering works for environmental reconstructions. The present investigation focuses on the morphological, biochemical toxicity and accumulation profile of heavy metals in *Spirodela polyrhiza* to various concentrations of sewage i.e 25, 50, 75 and 100% at regular intervals of 4 days upto 12 days. *Spirodela* showed visible symptoms like chlorosis, stunted growth, withering of roots and lower surface of leaf turns pink to whitish. However, the test plant shows luxurious growth at 25% of sewage. Biochemical estimations like total chlorophyll, protein and carbohydrate of the test plant shows luxurious growth at 25% sewage but biochemical activity decreased with increased concentrations of sewage and exposure durations, The accumulation profile of heavy metals is directly proportional to sewage concentration and exposure duration. It was observed that the accumulation potentiality in the test plant was maximum at 4 days exposure irrespective of concentrations, however, it remains marginal at remaining exposure duration.

INTRODUCTION

The indiscriminate disposal of industrial, municipal and agricultural wastes into the aquatic ecosystem are mainly responsible for environmental pollution, which contains excess amount of organic, inorganic material and forms sources of plant nutrients, in addition to the presence of variable amount of heavy metals (Brar *et, al;* 2000 and Bajguz 2011). The response of organisms depends on their inherent sensitivity of xenobiotics, Sensitive species fails to withstand the stress. The tolerant plant species survive, thrive well and multiply in polluted environment and serve as an indicator species for environmental quality. Aquatic macrophytes / microphytes possess tremendous accumulating potential to reduce the level of toxic metals from the sewage (Salt, *et.al*., 1998). The aquatic plants have the ability to accumulate the heavy metals &have been employed for the treatment of waste water (Rai, *et. al*., 2003; Wong *et. al.,* 1996). The bio removal process using aquatic plants often exhibits two stage uptake process: An initial step, reversible, metal binding process (biosorption), followed by a slow, irreversible, ion sequestration step (bioaccumulation) (Wilde and Benemann, 1993). In view of this, the present investigation evaluates the morphological, biochemical responses and accumulation of heavy metals in *Spirodela polyrhiza* from the sewage.

MATERIALS AND METHODS

The sewage was collected from Srinagar pond near to Karnataka University Dharwad, (India) was slightly brown in colour having foul smell. The analysis of physico-chemical parameters of sewage were carried out by using standard methods of APHA (1998). The test plant *Spirodela polyrhiza* (L) were sampled from Srinagar pond. The stock plants were maintained under the laboratory conditions and experiments were carried out in triplicates. The young *Spirodela* –test plants-were selected and acclimatized for two weeks in 4% Hoagland solution in the experimental pond of 10 lt capacity.

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50gms of fresh test plants were introduced simultaneously into each of the experimental ponds containing 25%, 50%,75% and 100% sewage and tap water (control) respectively. The experiments were conducted under standard physical conditions in green house of the Department of Botany, BLDEA's Degree College Jamkhandi. The plants were harvested at the end of 4, 8 and 12 days exposure and thoroughly washed with distilled water. The 25gm of plant material was harvested and used for the morphological observation and toxicity evaluation, for estimation of total chlorophyll, protein and carbohydrate content and also for the accumulation of heavy metals. Morphological Index Parameters (MIP) viz; root length leaf length and breadth were observed for 12 days at the interval of 4 days. Photographs of *Spirodela* treated with different concentrations of sewage were taken y using Canon's Power Shot G2 Digital camera. Fresh test plant samples were macerated in 100ml of 80% (v/v) chilled acetone by using pestle and morter. The extract was centrifused and supernatant was used for the estimation of total chlorophyll by Arnon method (1949), protein estimation by Lowary's method (1951) and carbohydrate estimation by Dubois method (1956). The heavy metal estimation of sewage was carried out by using standard method (Allen *et. al.*, 1974). The dry powder of one gram plant material one ml of sewage was digested using Gerhardt digestion unit. The digested sample was used for the estimation of heavy metals *viz,* Cadmium (Cd)-228.8nm, Lead (Pb)-217.00nm,Nickel (Ni)-232.0nm, Copper (Cu)-324.7nm; Zinc (Zn)-213.9nm, Manganese (Mn)-279.5nm and Iron (Fe)-248.3nm was done by Atomic Absorption Spectrometer(AAS)-(GBC-932 plus Australia) with air acetylene oxidising flame &metal hollow cathode lamp using their respective wavelength. Working standards [SISCOP-Chem-Bombay] were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values and ±SE from experimental data with three replicates. Data were subjected to three way ANOVA with two factor interaction to find out the significance between concentration and exposure duration, concentration and parameters and exposure duration and parameters. Further Dunet's test is also applied for multiple comparisons between control and other concentrations.

Table 1 Physico-Chemical characteristics of the sewage (Madihal)

Sl. No.	Parameters	Quantity
1	pH	8.08 ± 0.01
2	Electric Conductivity (EC)	1.28 mS ± 0.01
3	Total Dissolved Solids (TDS)	680.090 ± 5.50
4	Chloride	451.00 ± 4.48
5	Hardness	341.60 ± 3.82
6	Calcium (Ca)	95.00 ± 1.94
7	Magnesium (Mg)	73.00 ± 1.20
8	Dissolved Oxygen (DO)	3.60 ± 0.24
9	Sodium (Na)	141.00 ± 2.62
10	Potassium (K)	71.00 ± 1.0
11	Chemical Oxygen Demand (COD)	298.00 ± 3.72
12	Phosphates (PO_4)	2.11 ± 0.04
13	Sulphates ($S0_4$)	102.00 ± 4.92
14	Bicarbonates (HCO_3)	552.50 ± 4.84
15	Zinc (Zn)	498.00 ±4.00
16	Copper (Cu)	210.00 ± 5.3
17	Manganese (Mg)	443.00 ± 2.10
18	Iron (Fe)	1608.00 ± 5.02
19	Cadmium (Cd)	121.00 ± 1.04
20	Lead (Pb)	2103.00 ± 3.18
21	Nickel (Ni)	371.00 ± 1.42

Sl.No. 3 to 14 – values are expressed in mg/l
Sl.No. 15 to 21 – values are expressed in µg/l
mS – milli Siemens
Mean values ± SE

Table 2 Effect of sewage on morphology of *Spirodela polyrhiza*

Sewage Concentration (%)	Exposure duration								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	1.90 ± 0.047	1.866 ± 0.054	1.866 ± 0.072	0.633 ± 0.027	0.466 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.666 ± 0.027	0.533 ± 0.108
25	2.10 ± 0.124	2.70 ± 0.124	2.80 ± 0.047	0.833 ± 0.027	0.60 ± 0.047	0.866 ± 0.027	0. 26 ± 0.047	0.90 ± zero	0.733 ± 0.272
50	2.033 ± 0.054	2.433 ± 0.190	2.466 ± 0.118	0.733 ± 0.027	0.533 ± 0.072	0.733 ± 0.027	0.6 ± 0.0	7.666 ± 0.027	0.6 ± 0.047
75	1.933 ± 0.054	1.80 ± 0.047	1.40 ± 0.047	0.60 ± 0	0.047 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.533 ± 0.072	0.466 ± 0.027
100	1.866 ± 0.054	1.733 ± 0.054	1.266 ± 0.054	0.533 ± 0.272	0.5 ± 0.047	0.466 ± 0.027	0.43 ± 0.02	0.333 ± 0.027	0.3 ± 0.047

Values are expressed in cms
Mean values ± Standard Error

Table 3 Three way ANOVA with two factor interaction for the effect of sewage on biochemical constituents of *Spirodela polyrhiza*

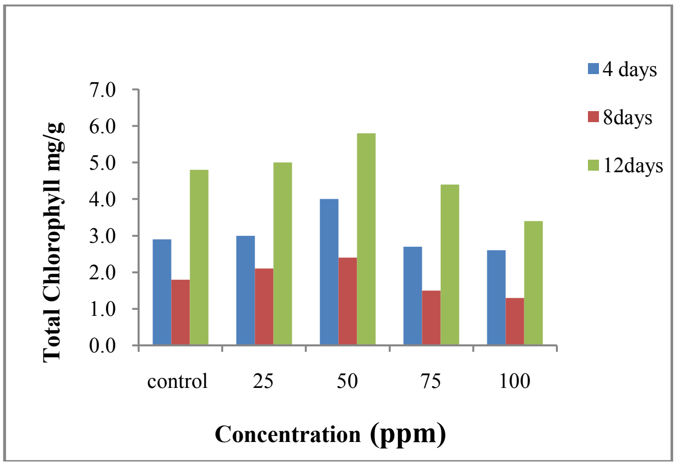
Sources of variation	Df	Sum of squares (SS)	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	8	42.282	5.285	1.187	0.365
Between concentration and parameters	8	193.221	24.153	5.425	0.002*
Between exposure and parameters	4	20.151	5.038	1.132	0.377

**Significant at $p < 0.01$ level

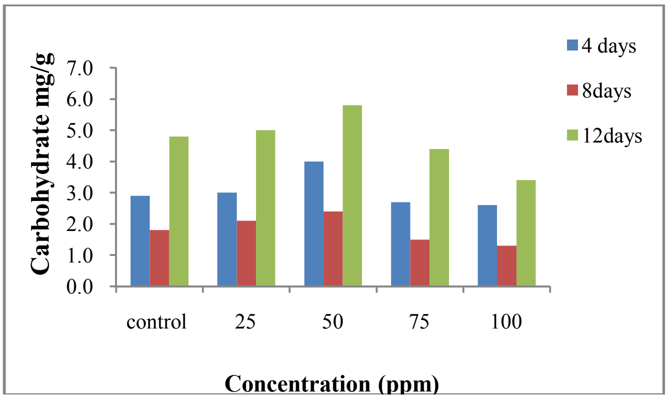
Table 4 Three way ANOVA with two factor interaction for the accumulation of heavy metals from the sewage by *Spirodela polyrhiza*

Sources of variation	Sum of squares (SS)	Df	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	532.75	8	66.594	1.99	0.068
Between concentration and parameters	132334.1	24	5513.92	165.04	0.00**
Between exposure and parameters	8507.13	12	708.92	21.21	0.000**

Significant at $p > 0.01$ level



A



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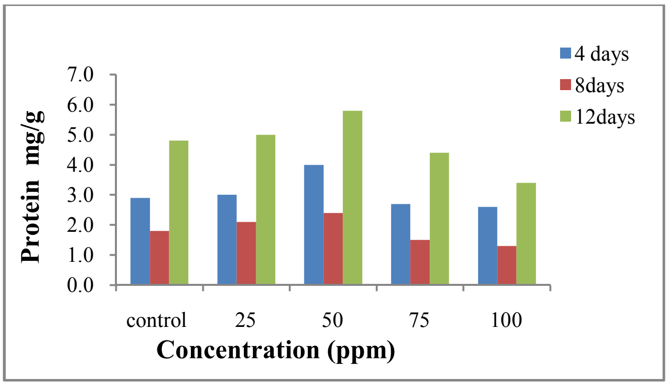
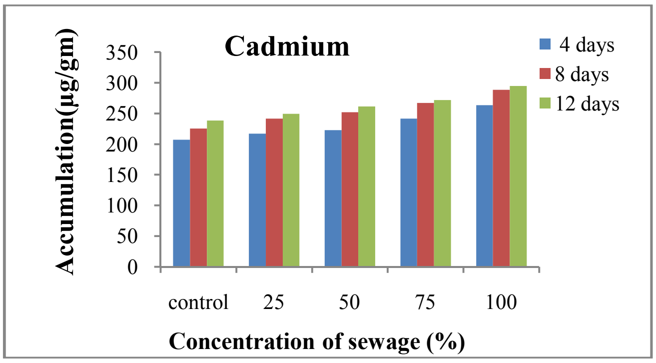


C

Fig 1 Biochemical effects of sewage on *Spirodela polyrhiza*
A) Total Chlorophyll B) Carbohydrate
B) Protein
C)



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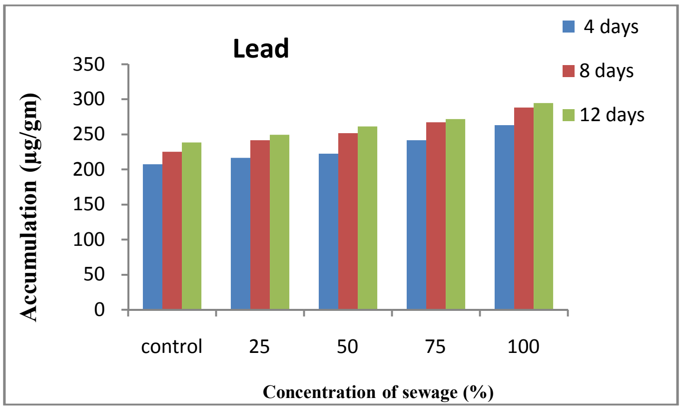

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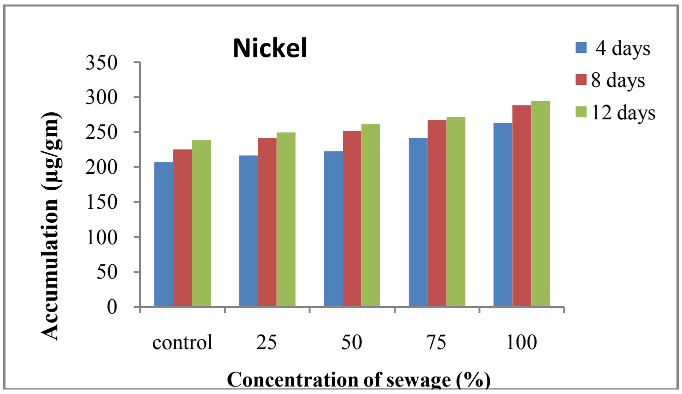
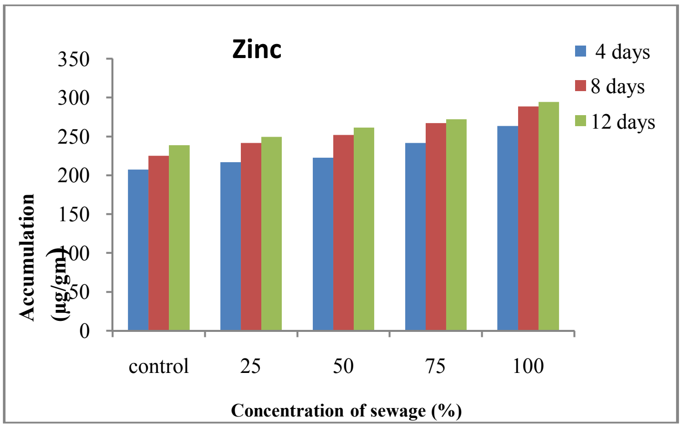
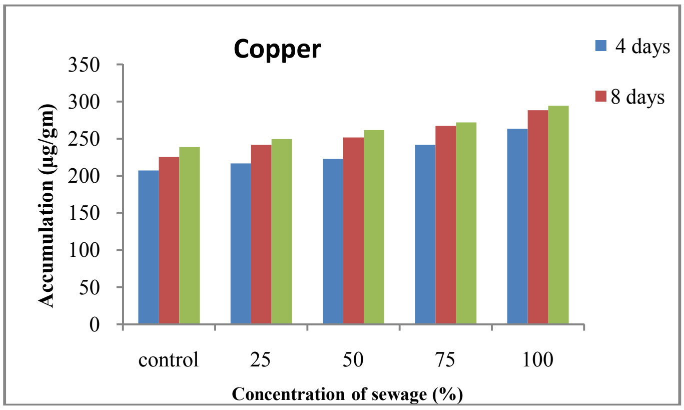


C)

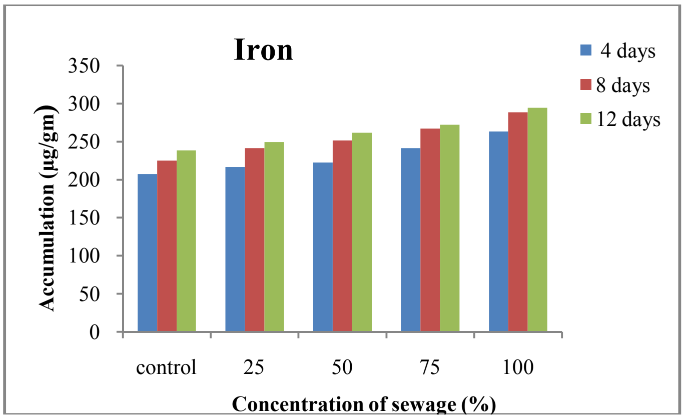


D)

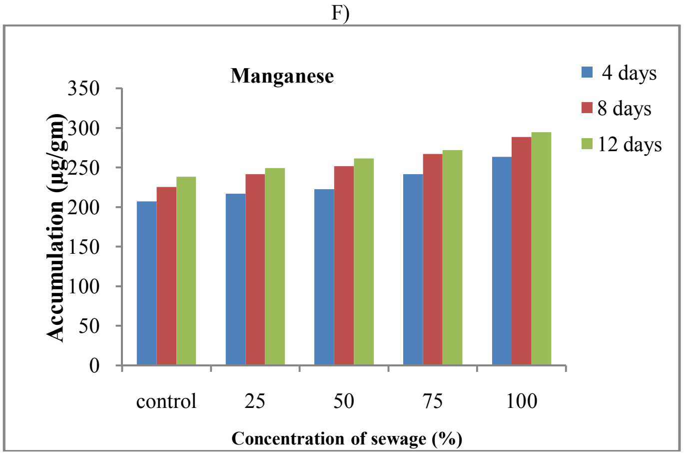
Fig 2 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*
A) Cadmium B) Lead C) Nickel D) Zinc



E)



F)



G)

Fig 3 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*
E) Copper F) Iron G) Manganese

RESULTS AND DISCUSSION

The results of physico-chemical and heavy metal analysis of sewage are present in Table -1.The sewage is slightly brown in colour with foul smell.

Toxicity Effect of Sewage Morphology

Morphometric assay is one of the quantitative tool for the assessments present in the sewage was measured by using Morphological Index Parameters (MIP). The test plant showed luxuriant growth in the laminal length and breadth at 25% sewage and it was found to promote the laminal length by 0.833 ± 0.027 cm, 0.90 ± zero cm at 4 and 12 days exposure duration and breadth by 0.60 ± 0.047 cm, 0.733 ± 0.272 cm, similarly root length by 2.10 ± 0.124 cm, 2.80 ± 0.047cm at the same exposure duration. However, the 100% sewage severely inhibit the laminal length by 0.533 ± 0.272 cm and 0.333 ± 0.027cm and breadth to about 0.5 ± 0.047 cm and 0.3 ± 0.047 cm at 4 and 12 days exposure duration. Similarly root inhibition was also noticed to the extent of 1.866 ± 0.054cm and 1.266 ± 0.054 cm at the same exposure duration. (Table 2). The plants require some of the heavy metals *viz*, Zn, Cu, Ni, Mn etc as essential macro-nutrients and are very sensitive to metabolic activities at higher concentrations (Reeves and Baker 2000)

The experimental plants shows the normal and healthy growth at lower concentration of sewage (25%) The similar observations were made by Pandit *et. al.,* (1996) in the germination of seedlings growth of *Sorghum* at 25% dairy effluent, Singh *et, al.,* (2005) also showed that 25% sugar factory effluent rich in nutrients supports optimal growth of *Potomegaton pectinatus*. In present investigation the higher concentration of sewage (100%) exhibits inhibitory effects in the test plant .The *Spirodela* shows toxic symptoms such as necrosis, yellowish, white leaves, degeneration of the leaves and disappearance of roots during 12 days exposure duration. The excess accumulation of metals in different tissues of the is responsible for morphological changes due to the interference of absorbed metal ions in the metabolism (Satyakala and Jamil, 1997).The inhibition of root growth is mainly due to the direct contact of root tip meristem with heavy metals of the experimental pond. These heavy metal brings considerable change in the rate of metabolic process of cells including nucleic acid synthesis, protein synthesis etc (Nag *et, al.,* 1981).Similar observation were also made by Marawari and Sharma (2005) in *Raphanes sativus* treated with textile waste water.

Three way ANOVA with two factor interaction for the effect of sewage on the length and breadth and also root length between root exposure and concentration is significant at 1% (P>0.01).

Toxicity Effect of Sewage on Biochemical Parameters

Biochemical changes in *Spirodela* in response to sewage are presented in the fig.(1). From the data, it is evident that the total chlorophyll present in *Spirodela* decrease with an increase in the concentration of sewage. The 25%. sewage was found to promote the synthesis of chlorophyll by 0.623 ± 0.12mg/gm (27-40%) at 4 days and 0.697 ± 0.24 mg/gm at 12 days in comparison to control. However, 100% sewage was found to inhibit the chlorophyll synthesis by 0.474 ± 0.08mg/gm (3.06%) and 0.371 ± 0.12 mg/gm (46.77%) respectively during 4 and 12 days exposure duration in comparison to control. Biochemical response of aquatic macrophyte to the toxicity of different heavy metals in an expression of their quality and quantity of the biochemical constituents. The interference of the heavy metals in cellular mechanisms by altering the structure of enzymes by changing the configuration of enzyme molecule by competitive inhibition of heavy metals. This either enhances or inhibits the synthesis of biomolecules (Brar *et, al.,* 2000). In the present investigation the experimental plant grown in 25% sewage found to promote the synthesis of chlorophyll from 0.623 ± 8.12 mg/gm (27-40%) and 0.697 ± 0.24 mg/gm, (34-35%) in 4 and 12 days exposure respectively. The increase in total chlorophyll content may be due to the optimal nutrient level which favoured the chlorophyll synthesis (Bendra and Mishra, 1983). The chlorophyll stimulation is associated with formation of phytochelatins (PCs) , plays an important role in detoxification (Prasad, 2004; Sibihil *et, al.,* 2012,).

However, the higher concentration of sewage was found to inhibit chlorophyll and directly proportional to the exposure. The 100% sewage was found to inhibit the chlorophyll in the experimental plant to about 3.06% and 46.77% at 4 and 12 days exposure respectively in comparison to control . The heavy metals present in the sewage was responsible for the degradation of photosynthetic pigments (Vajpayee *et, al.,* 2000), which ultimately causes deficiency in light harvesting capacity (Quzounidou, 1996). According to Prasad and Prasad (1987) the heavy metals are the potent inhibitors of biosynthesis of chlorophyll. The major sites of inhibition are in the formation of proteolytic phytochelatin (PC) helide reductase complex and synthesis of δ-aminolevulinic acid dehydrogenase (δ ALAD),chloroplast enzyme, which catalyses the pathway of porphobilinogen (PBG)synthesis for δ-aminolevulinic acid (ALA) (Prasad and Prasad 1987: Sing *et, al.,* 2005; Sibihi *et, al.,* 2012).

In the present investigation the 25% and 50% sewage promotes synthesis of carbohydrates. The 50% sewage promotes synthesis of carbohydrate. A remarkable carbohydrate content of 34 ± 0.12mg/gm (54.54%) was observed at 50% sewage during 12 days exposure in comparison to control. However, the carbohydrate inhibition at 100% sewage amounts to 17.02 ± 0.14mg/gm (5.55%) at 4 days and 12.0 ± 1.24mg/gm (45.45%)

at 12 days exposure duration. It was reported that the accumulation of carbohydrate in algal cells, Viz*; Anabaena* sps, *Fischerella* sps grown in highly diluted effluent and carbohydrate content is directly proportional to chlorophyll content (Renuga, 2005). The increased concentration of sewage has impact on photosynthetic activity, as the heavy metals *Viz,* Pb, Ni, Cd and Cu damages the chloroplast structure, hinders the photosynthetic assimilation (Hasan *et, al.,* 2009).

The lower concentrations of sewage , 25% and 50% found to promote the protein synthesis .The 50% sewage was also found to promote protein synthesis by 4.0 ± 0.18 mg/gm at 4 days and 5.8 ± 1.12mg/gm at an exposure duration of 12 days, however, 100% sewage was found to inhibit the protein by 2.6 ± 0.12 mg/gm at 4 days and it promotes synthesis by 3.4 ± 0.14 mg/gm during an exposure duration of 12 days. In the present investigation 25% and 50% sewage promotes the protein synthesis, but 50% more promotive by 37.93% to 41.66% at 4 and 12 days exposure in comparison to control. Similar observation was made in seedlings of *Oryza sativa* at 5% chloroalkali factory effluent (Radha and Panigrahi, 1998). The 75% and 100% sewage exhibits inhibitory effects on protein synthesis in test plant upto 8 days, however, later there will be augmentation of protein synthesis . The protein at 100% sewage is 2.8 ± 0.16 mg/g, (9.67 %), 1.8 ± 0.16 mg/g, (5.82 %) and 4.6 ± 0.12 mg/g (16.68 %) at 4, 8 and 12 days exposure. After 8 days exposure, the 100% sewage was found to augment the protein synthesis from 1.8 ± 0.16 mg/g to 4.6 ± 0.12 mg/gm was noticed due to synthesis of stress proteins or metallothionines, but later declines due to toxic effect of heavy metal on protein synthesis due to increased activity of protease, blockage of –SH group of protein. Similar observations were made by Ali *et, al., (*2003) in *Salix acomophylla* using heavy metals like Cu, Ni and Pb, it is demonstrated that the cations and anions present in the sewage affects the quality of both DNA and RNA, ultimately leads to the reduction of protein synthesis (Phalsson,1989; Marowari, *et, al.,* 2005).

Three way ANOVA with two factor interaction among the concentration, exposure duration and parameters was applied to know the association between concentration and exposure duration, concentration and parameters and exposure duration and parameters. From the data it is clear that there is (P<0.01 level) a significant association between concentration and parameters. The result reveals that the concentration and parameters are highly significant, whereas other factors are related but not significant .(Table 3).

Profile of Metal Accumulation

Spirodela showed high amelioration potential of heavy metals *Viz*, Pb, Cd, Zn, Ni, Cu,Fe and Mn etc by accumulation in its tissues (Fig 2 and 3). It is apparent from the present study that the accumulation of metals was maximum during four days exposure and thereafter marginal increase in accumulation of metals, *Spirodela* exhibit high degree of accumulation of Cd, Ni, Cu, Fe followed by Pb.At 25% sewage the *Spirodela* found to accumulate Cd to the extent of 2.00± 1.02 µg/gm and 2.75± 0.12 µg/m at 4 and 12 days exposure respectively. The phytoaccumulation is maximum (3.75±1.02 µg/m) in the plants grown in 100%. sewage during 12days exposure in comparison to control (1.75 ± 0.12 µg/m), Ni accumulation is 34.50 ± 0.12 µg/m and 44.0 ± 1.12 µg/m at 25% and 100% sewage respectively.

Iron accumulation in test plant vary 518.25 ± 1.12 µg/gm to 575.25 ± 1.12 µg/gm in 25% and 100% sewage respectively in comparison to control (258.25 ± 1.10 µg/gm) during 12 days exposure .The accumulation of Cu from the sewage 64.75 ± 0.12 µg/gm and 70.25 ± 1.10 µg/gm from 50% and 100% sewage respectively during 12 days exposure in comparison to control (52.25 ± 1.10 µg/gm). Similarly, Zn accumulation at 100% sewage is 70.25 ± 0.12 µg/gm during 12 days exposure compared to control (46.75 ± 1.12 µg/gm).

Three way ANOVA represents significant association at P<0.01 level between concentration and parameters and exposure and parameters. This represents the high significant in metal accumulation but other factors are also related, but at significant level (P>0.05) Two way ANOVA represents concentrations and exposure duration are significant at 0.01 level (Table-4) and Dunet's test also reveals that the concentrations are significantly differ with control.

Sewage containing heavy metals poses multiple hazards (Berti and Cunningham, 2000) to aquatic flora and fauna. Aquatic plants have capability to accumulate heavy metals of from the media and thereby, cleaning the environment (Kara,2003; Singh *et, al.,* 2005). The data reveals that the order of accumulation of heavy metals from the sewage is as follows:

Fe > Cd > Pb > Zn > Ni > Cu > Mn

The similar observations were made in *Lemna minor* and *Phragmites karka*, was high at lower concentration of waste water and absorption capacity of the plant is marginal at subsequent concentrations and exposure duration (Pandey and Pandey, 2006; Phetsombat *et, al.,* 2006). It is evident from the present investigation that the accumulation of metals was maximum at 4 days exposure and later it was marginal, Thus, *Spirodela polyrhiza* is found to be a suitable candidate for toxicity evaluation and is used for the remediation of heavy metals from the aquatic ecosystem and environmental cleaning.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Degree College, Jamkhandi (India), Research and Development Centre, Bharthiar University, Coimbatore (Tamil Nadu), Dept.of Botany, Karnataka University Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also greateful to authors/editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed.

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ISSN: 0976-3031

Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 07 (A), pp. 39115-39120, July, 2020

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

BIOACCUMULATION OF XENOBIOTICS FROM SEWAGE BY AQUATIC MACROPHYTE

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1107.5444

ARTICLE INFO

Article History:

Received 06th April, 2020
Received in revised form 14th May, 2020
Accepted 23rd June, 2020
Published online 28th July, 2020

Key Words:

Heavy metals, accumulation, sewage, toxicity, biochemical parameters.

ABSTRACT

Increasing urbanization, industrialization, and over population and anthropogenic activities have contributed huge quantities, industrial and domestic waste water, which contains huge quantities of xenobiotics that leads to undesirable changes of the environment.

The *xenobiotics* disrupts the food chain and some toxicants are lethal even a lower concentrations. The prevailing purification technologies used for the removal of contaminants from the sewage are not only costly but causes negative impact on ecosystem subsequently .The aquatic plants have the potentiality to accumulate xenobiotics, as they were tolerant and able to withstand the pollution stress. They serve as a tool for the remediation of xenobiotics from the aquatic ecosystem. Phytoremediation is an emerging “Green Bioengineering Technology” and this concept is cheaper and alternative that hardly cost civil engineering works for environmental reconstructions. The present investigation focuses on the morphological, biochemical toxicity and accumulation profile of heavy metals in *Spirodela polyrhiza* to various concentrations of sewage i.e 25, 50, 75 and 100% at regular intervals of 4 days upto 12 days. *Spirodela* showed visible symptoms like chlorosis, stunted growth, withering of roots and lower surface of leaf turns pink to whitish. However, the test plant shows luxurious growth at 25% of sewage. Biochemical estimations like total chlorophyll, protein and carbohydrate of the test plant shows luxurious growth at 25% sewage but biochemical activity decreased with increased concentrations of sewage and exposure durations, The accumulation profile of heavy metals is directly proportional to sewage concentration and exposure duration. It was observed that the accumulation potentiality in the test plant was maximum at 4 days exposure irrespective of concentrations, however, it remains marginal at remaining exposure duration.

INTRODUCTION

The indiscriminate disposal of industrial, municipal and agricultural wastes into the aquatic ecosystem are mainly responsible for environmental pollution, which contains excess amount of organic, inorganic material and forms sources of plant nutrients, in addition to the presence of variable amount of heavy metals (Brar *et, al;* 2000 and Bajguz 2011). The response of organisms depends on their inherent sensitivity of xenobiotics, Sensitive species fails to withstand the stress. The tolerant plant species survive, thrive well and multiply in polluted environment and serve as an indicator species for environmental quality. Aquatic macrophytes / microphytes possess tremendous accumulating potential to reduce the level of toxic metals from the sewage (Salt, *et.al*., 1998). The aquatic plants have the ability to accumulate the heavy metals &have been employed for the treatment of waste water (Rai, *et. al*., 2003; Wong *et. al.,* 1996). The bio removal process using aquatic plants often exhibits two stage uptake process: An initial step, reversible, metal binding process (biosorption), followed by a slow, irreversible, ion sequestration step (bioaccumulation) (Wilde and Benemann, 1993). In view of this, the present investigation evaluates the morphological, biochemical responses and accumulation of heavy metals in *Spirodela polyrhiza* from the sewage.

MATERIALS AND METHODS

The sewage was collected from Srinagar pond near to Karnataka University Dharwad, (India) was slightly brown in colour having foul smell. The analysis of physico-chemical parameters of sewage were carried out by using standard methods of APHA (1998). The test plant *Spirodela polyrhiza* (L) were sampled from Srinagar pond. The stock plants were maintained under the laboratory conditions and experiments were carried out in triplicates. The young *Spirodela* –test plants-were selected and acclimatized for two weeks in 4% Hoagland solution in the experimental pond of 10 lt capacity.

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50gms of fresh test plants were introduced simultaneously into each of the experimental ponds containing 25%, 50%,75% and 100% sewage and tap water (control) respectively. The experiments were conducted under standard physical conditions in green house of the Department of Botany, BLDEA's Degree College Jamkhandi. The plants were harvested at the end of 4, 8 and 12 days exposure and thoroughly washed with distilled water. The 25gm of plant material was harvested and used for the morphological observation and toxicity evaluation, for estimation of total chlorophyll, protein and carbohydrate content and also for the accumulation of heavy metals. Morphological Index Parameters (MIP) viz; root length leaf length and breadth were observed for 12 days at the interval of 4 days. Photographs of *Spirodela* treated with different concentrations of sewage were taken y using Canon's Power Shot G2 Digital camera. Fresh test plant samples were macerated in 100ml of 80% (v/v) chilled acetone by using pestle and morter. The extract was centrifused and supernatant was used for the estimation of total chlorophyll by Arnon method (1949), protein estimation by Lowary's method (1951) and carbohydrate estimation by Dubois method (1956). The heavy metal estimation of sewage was carried out by using standard method (Allen *et. al.*, 1974). The dry powder of one gram plant material one ml of sewage was digested using Gerhardt digestion unit. The digested sample was used for the estimation of heavy metals *viz,* Cadmium (Cd)-228.8nm, Lead (Pb)-217.00nm,Nickel (Ni)-232.0nm, Copper (Cu)-324.7nm; Zinc (Zn)-213.9nm, Manganese (Mn)-279.5nm and Iron (Fe)-248.3nm was done by Atomic Absorption Spectrometer(AAS)-(GBC-932 plus Australia) with air acetylene oxidising flame &metal hollow cathode lamp using their respective wavelength. Working standards [SISCOP-Chem-Bombay] were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values and ±SE from experimental data with three replicates. Data were subjected to three way ANOVA with two factor interaction to find out the significance between concentration and exposure duration, concentration and parameters and exposure duration and parameters. Further Dunet's test is also applied for multiple comparisons between control and other concentrations.

Table 1 Physico-Chemical characteristics of the sewage (Madihal)

Sl. No.	Parameters	Quantity
1	pH	8.08 ± 0.01
2	Electric Conductivity (EC)	1.28 mS ± 0.01
3	Total Dissolved Solids (TDS)	680.090 ± 5.50
4	Chloride	451.00 ± 4.48
5	Hardness	341.60 ± 3.82
6	Calcium (Ca)	95.00 ± 1.94
7	Magnesium (Mg)	73.00 ± 1.20
8	Dissolved Oxygen (DO)	3.60 ± 0.24
9	Sodium (Na)	141.00 ± 2.62
10	Potassium (K)	71.00 ± 1.0
11	Chemical Oxygen Demand (COD)	298.00 ± 3.72
12	Phosphates (PO_4)	2.11 ± 0.04
13	Sulphates ($S0_4$)	102.00 ± 4.92
14	Bicarbonates (HCO_3)	552.50 ± 4.84
15	Zinc (Zn)	498.00 ±4.00
16	Copper (Cu)	210.00 ± 5.3
17	Manganese (Mg)	443.00 ± 2.10
18	Iron (Fe)	1608.00 ± 5.02
19	Cadmium (Cd)	121.00 ± 1.04
20	Lead (Pb)	2103.00 ± 3.18
21	Nickel (Ni)	371.00 ± 1.42

Sl.No. 3 to 14 – values are expressed in mg/l
Sl.No. 15 to 21 – values are expressed in µg/l
mS – milli Siemens
Mean values ± SE

Table 2 Effect of sewage on morphology of *Spirodela polyrhiza*

Sewage Concentration (%)	**Exposure duration**								
	4	**8**	**12**	**4**		**8**		**12**	
	Root length			**Leaf size**					
				Length	**Breadth**	**Length**	**Breadth**	**Length**	**Breadth**
Control 0	1.90 ± 0.047	1.866 ± 0.054	1.866 ± 0.072	0.633 ± 0.027	0.466 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.666 ± 0.027	0.533 ± 0.108
25	2.10 ± 0.124	2.70 ± 0.124	2.80 ± 0.047	0.833 ± 0.027	0.60 ± 0.047	0.866 ± 0.027	0. 26 ± 0.047	0.90 ± zero	0.733 ± 0.272
50	2.033 ± 0.054	2.433 ± 0.190	2.466 ± 0.118	0.733 ± 0.027	0.533 ± 0.072	0.733 ± 0.027	0.6 ± 0.0	7.666 ± 0.027	0.6 ± 0.047
75	1.933 ± 0.054	1.80 ± 0.047	1.40 ± 0.047	0.60 ± 0	0.047 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.533 ± 0.072	0.466 ± 0.027
100	1.866 ± 0.054	1.733 ± 0.054	1.266 ± 0.054	0.533 ± 0.272	0.5 ± 0.047	0.466 ± 0.027	0.43 ± 0.02	0.333 ± 0.027	0.3 ± 0.047

Values are expressed in cms
Mean values ± Standard Error

Table 3 Three way ANOVA with two factor interaction for the effect of sewage on biochemical constituents of *Spirodela polyrhiza*

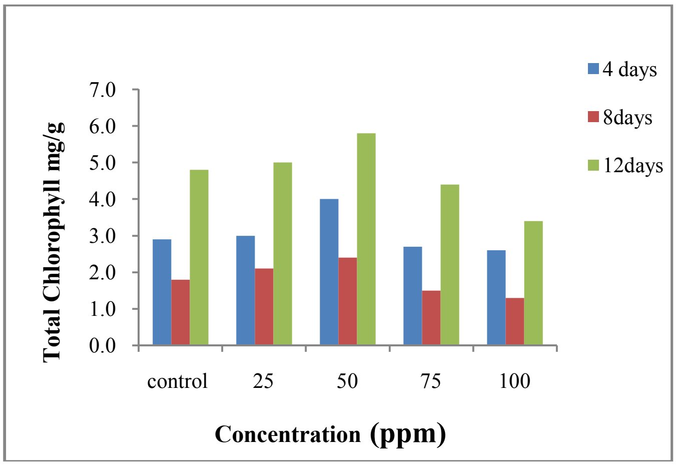
Sources of variation	Df	Sum of squares (SS)	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	8	42.282	5.285	1.187	0.365
Between concentration and parameters	8	193.221	24.153	5.425	0.002*
Between exposure and parameters	4	20.151	5.038	1.132	0.377

**Significant at $p < 0.01$ level

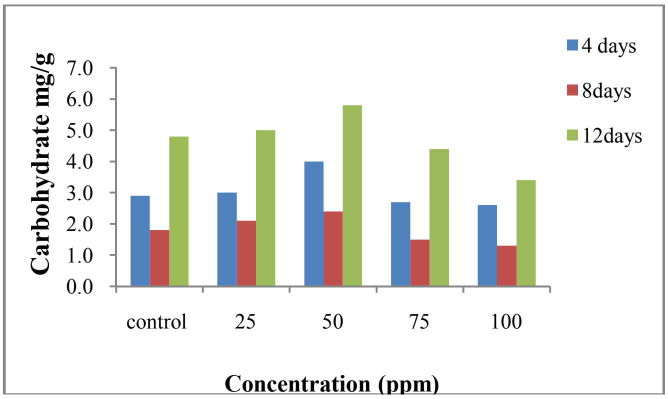
Table 4 Three way ANOVA with two factor interaction for the accumulation of heavy metals from the sewage by *Spirodela polyrhiza*

Sources of variation	Sum of squares (SS)	Df	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	532.75	8	66.594	1.99	0.068
Between concentration and parameters	132334.1	24	5513.92	165.04	0.00**
Between exposure and parameters	8507.13	12	708.92	21.21	0.000**

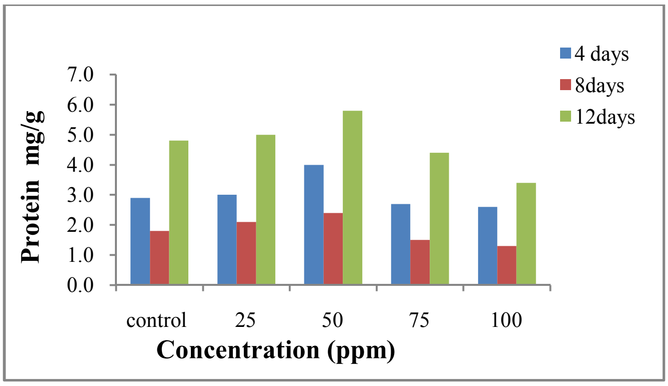
Significant at $p > 0.01$ level



A

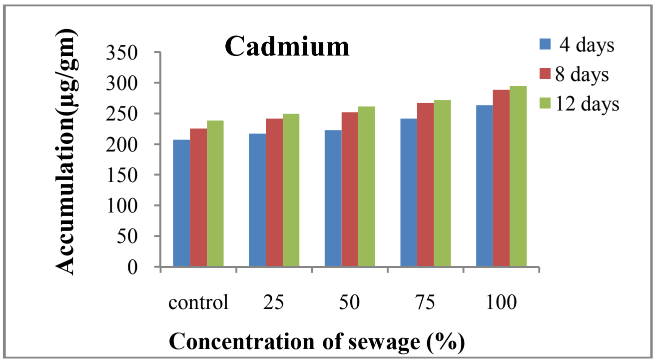


B

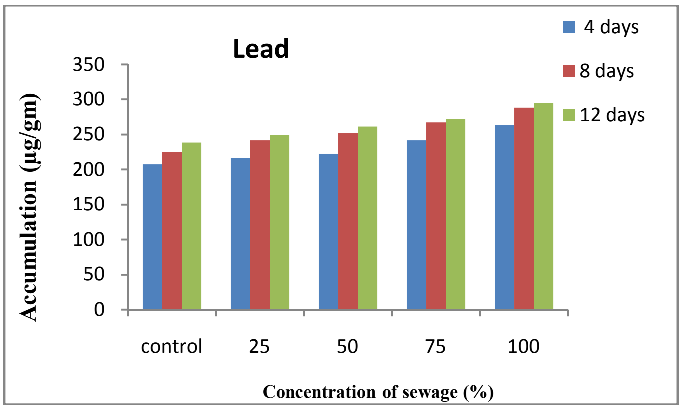


C

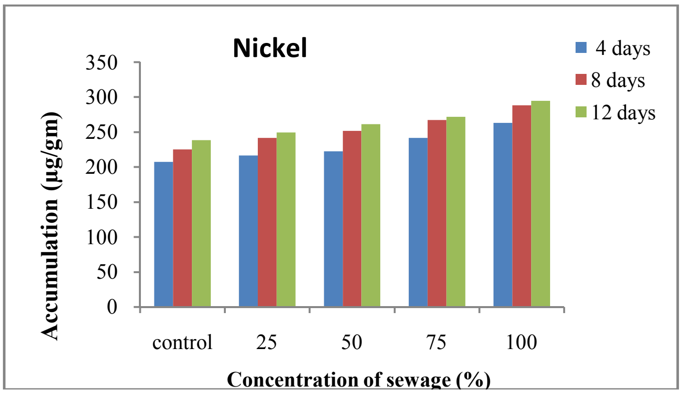
Fig 1 Biochemical effects of sewage on *Spirodela polyrhiza*
A) Total Chlorophyll B) Carbohydrate
B) Protein
C)



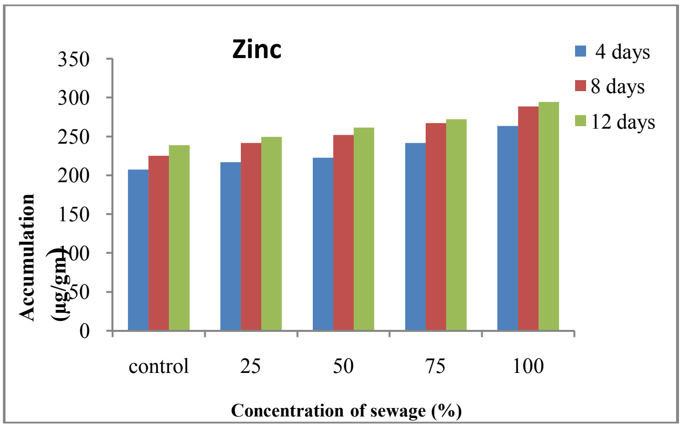
A



B



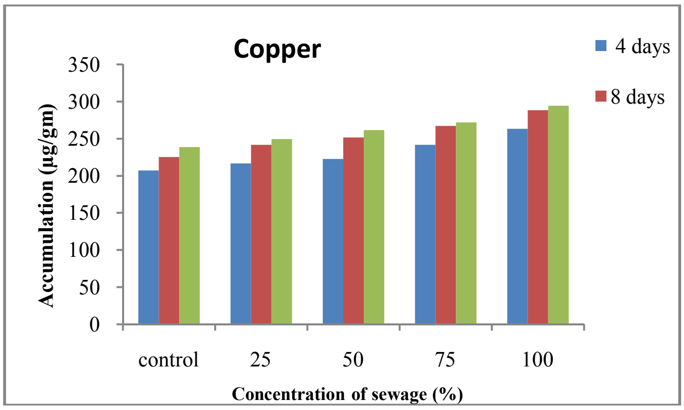
C)



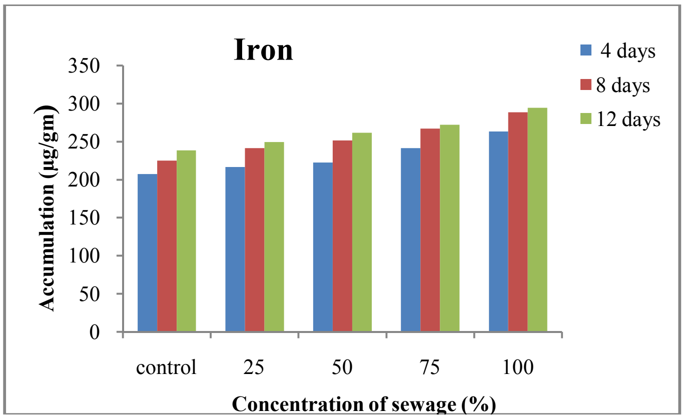
D)

Fig 2 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*

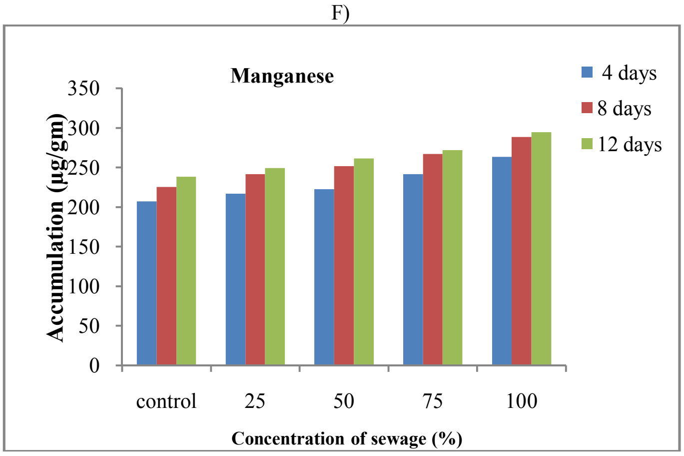
A) Cadmium B) Lead C) Nickel D) Zinc



E)



F)



G)

Fig 3 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*
E) Copper F) Iron G) Manganese

RESULTS AND DISCUSSION

The results of physico-chemical and heavy metal analysis of sewage are present in Table -1.The sewage is slightly brown in colour with foul smell.

Toxicity Effect of Sewage Morphology

Morphometric assay is one of the quantitative tool for the assessments present in the sewage was measured by using Morphological Index Parameters (MIP). The test plant showed luxuriant growth in the laminal length and breadth at 25% sewage and it was found to promote the laminal length by 0.833 ± 0.027 cm, 0.90 ± zero cm at 4 and 12 days exposure duration and breadth by 0.60 ± 0.047 cm, 0.733 ± 0.272 cm, similarly root length by 2.10 ± 0.124 cm, 2.80 ± 0.047cm at the same exposure duration. However, the 100% sewage severely inhibit the laminal length by 0.533 ± 0.272 cm and 0.333 ± 0.027cm and breadth to about 0.5 ± 0.047 cm and 0.3 ± 0.047 cm at 4 and 12 days exposure duration. Similarly root inhibition was also noticed to the extent of 1.866 ± 0.054cm and 1.266 ± 0.054 cm at the same exposure duration. (Table 2). The plants require some of the heavy metals *viz*, Zn, Cu, Ni, Mn etc as essential macro-nutrients and are very sensitive to metabolic activities at higher concentrations (Reeves and Baker 2000)

The experimental plants shows the normal and healthy growth at lower concentration of sewage (25%) The similar observations were made by Pandit *et. al.,* (1996) in the germination of seedlings growth of *Sorghum* at 25% dairy effluent, Singh *et, al.,* (2005) also showed that 25% sugar factory effluent rich in nutrients supports optimal growth of *Potomegaton pectinatus*. In present investigation the higher concentration of sewage (100%) exhibits inhibitory effects in the test plant .The *Spirodela* shows toxic symptoms such as necrosis, yellowish, white leaves, degeneration of the leaves and disappearance of roots during 12 days exposure duration. The excess accumulation of metals in different tissues of the is responsible for morphological changes due to the interference of absorbed metal ions in the metabolism (Satyakala and Jamil, 1997).The inhibition of root growth is mainly due to the direct contact of root tip meristem with heavy metals of the experimental pond. These heavy metal brings considerable change in the rate of metabolic process of cells including nucleic acid synthesis, protein synthesis etc (Nag *et, al.,* 1981).Similar observation were also made by Marawari and Sharma (2005) in *Raphanes sativus* treated with textile waste water.

Three way ANOVA with two factor interaction for the effect of sewage on the length and breadth and also root length between root exposure and concentration is significant at 1% (P>0.01).

Toxicity Effect of Sewage on Biochemical Parameters

Biochemical changes in *Spirodela* in response to sewage are presented in the fig.(1). From the data, it is evident that the total chlorophyll present in *Spirodela* decrease with an increase in the concentration of sewage. The 25%. sewage was found to promote the synthesis of chlorophyll by 0.623 ± 0.12mg/gm (27-40%) at 4 days and 0.697 ± 0.24 mg/gm at 12 days in comparison to control. However, 100% sewage was found to inhibit the chlorophyll synthesis by 0.474 ± 0.08mg/gm (3.06%) and 0.371 ± 0.12 mg/gm (46.77%) respectively during 4 and 12 days exposure duration in comparison to control. Biochemical response of aquatic macrophyte to the toxicity of different heavy metals in an expression of their quality and quantity of the biochemical constituents. The interference of the heavy metals in cellular mechanisms by altering the structure of enzymes by changing the configuration of enzyme molecule by competitive inhibition of heavy metals. This either enhances or inhibits the synthesis of biomolecules (Brar *et, al.,* 2000). In the present investigation the experimental plant grown in 25% sewage found to promote the synthesis of chlorophyll from 0.623 ± 8.12 mg/gm (27-40%) and 0.697 ± 0.24 mg/gm, (34-35%) in 4 and 12 days exposure respectively. The increase in total chlorophyll content may be due to the optimal nutrient level which favoured the chlorophyll synthesis (Bendra and Mishra, 1983). The chlorophyll stimulation is associated with formation of phytochelatins (PCs) , plays an important role in detoxification (Prasad, 2004; Sibihil *et, al.,* 2012,).

However, the higher concentration of sewage was found to inhibit chlorophyll and directly proportional to the exposure. The 100% sewage was found to inhibit the chlorophyll in the experimental plant to about 3.06% and 46.77% at 4 and 12 days exposure respectively in comparison to control . The heavy metals present in the sewage was responsible for the degradation of photosynthetic pigments (Vajpayee *et, al.,* 2000), which ultimately causes deficiency in light harvesting capacity (Quzounidou, 1996). According to Prasad and Prasad (1987) the heavy metals are the potent inhibitors of biosynthesis of chlorophyll. The major sites of inhibition are in the formation of proteolytic phytochelatin (PC) helide reductase complex and synthesis of δ-aminolevulinic acid dehydrogenase (δ ALAD),chloroplast enzyme, which catalyses the pathway of porphobilinogen (PBG)synthesis for δ-aminolevulinic acid (ALA) (Prasad and Prasad 1987: Sing *et, al.,* 2005; Sibihi *et, al.,* 2012).

In the present investigation the 25% and 50% sewage promotes synthesis of carbohydrates. The 50% sewage promotes synthesis of carbohydrate. A remarkable carbohydrate content of 34 ± 0.12mg/gm (54.54%) was observed at 50% sewage during 12 days exposure in comparison to control. However, the carbohydrate inhibition at 100% sewage amounts to 17.02 ± 0.14mg/gm (5.55%) at 4 days and 12.0 ± 1.24mg/gm (45.45%)

at 12 days exposure duration. It was reported that the accumulation of carbohydrate in algal cells, Viz*; Anabaena* sps, *Fischerella* sps grown in highly diluted effluent and carbohydrate content is directly proportional to chlorophyll content (Renuga, 2005). The increased concentration of sewage has impact on photosynthetic activity, as the heavy metals *Viz,* Pb, Ni, Cd and Cu damages the chloroplast structure, hinders the photosynthetic assimilation (Hasan *et, al.,* 2009).

The lower concentrations of sewage , 25% and 50% found to promote the protein synthesis .The 50% sewage was also found to promote protein synthesis by 4.0 ± 0.18 mg/gm at 4 days and 5.8 ± 1.12mg/gm at an exposure duration of 12 days, however, 100% sewage was found to inhibit the protein by 2.6 ± 0.12 mg/gm at 4 days and it promotes synthesis by 3.4 ± 0.14 mg/gm during an exposure duration of 12 days. In the present investigation 25% and 50% sewage promotes the protein synthesis, but 50% more promotive by 37.93% to 41.66% at 4 and 12 days exposure in comparison to control. Similar observation was made in seedlings of *Oryza sativa* at 5% chloroalkali factory effluent (Radha and Panigrahi, 1998). The 75% and 100% sewage exhibits inhibitory effects on protein synthesis in test plant upto 8 days, however, later there will be augmentation of protein synthesis . The protein at 100% sewage is 2.8 ± 0.16 mg/g, (9.67 %), 1.8 ± 0.16 mg/g, (5.82 %) and 4.6 ± 0.12 mg/g (16.68 %) at 4, 8 and 12 days exposure. After 8 days exposure, the 100% sewage was found to augment the protein synthesis from 1.8 ± 0.16 mg/g to 4.6 ± 0.12 mg/gm was noticed due to synthesis of stress proteins or metallothionines, but later declines due to toxic effect of heavy metal on protein synthesis due to increased activity of protease, blockage of –SH group of protein. Similar observations were made by Ali *et, al., (*2003) in *Salix acomophylla* using heavy metals like Cu, Ni and Pb, it is demonstrated that the cations and anions present in the sewage affects the quality of both DNA and RNA, ultimately leads to the reduction of protein synthesis (Phalsson,1989; Marowari, *et, al.,* 2005).

Three way ANOVA with two factor interaction among the concentration, exposure duration and parameters was applied to know the association between concentration and exposure duration, concentration and parameters and exposure duration and parameters. From the data it is clear that there is (P<0.01 level) a significant association between concentration and parameters. The result reveals that the concentration and parameters are highly significant, whereas other factors are related but not significant .(Table 3).

Profile of Metal Accumulation

Spirodela showed high amelioration potential of heavy metals *Viz*, Pb, Cd, Zn, Ni, Cu,Fe and Mn etc by accumulation in its tissues (Fig 2 and 3). It is apparent from the present study that the accumulation of metals was maximum during four days exposure and thereafter marginal increase in accumulation of metals, *Spirodela* exhibit high degree of accumulation of Cd, Ni, Cu, Fe followed by Pb.At 25% sewage the *Spirodela* found to accumulate Cd to the extent of 2.00± 1.02 µg/gm and 2.75± 0.12 µg/m at 4 and 12 days exposure respectively. The phytoaccumulation is maximum (3.75±1.02 µg/m) in the plants grown in 100%. sewage during 12days exposure in comparison to control (1.75 ± 0.12 µg/m), Ni accumulation is 34.50 ± 0.12 µg/m and 44.0 ± 1.12 µg/m at 25% and 100% sewage respectively.

Iron accumulation in test plant vary 518.25 ± 1.12 µg/gm to 575.25 ± 1.12 µg/gm in 25% and 100% sewage respectively in comparison to control (258.25 ± 1.10 µg/gm) during 12 days exposure .The accumulation of Cu from the sewage 64.75 ± 0.12 µg/gm and 70.25 ± 1.10 µg/gm from 50% and 100% sewage respectively during 12 days exposure in comparison to control (52.25 ± 1.10 µg/gm). Similarly, Zn accumulation at 100% sewage is 70.25 ± 0.12 µg/gm during 12 days exposure compared to control (46.75 ± 1.12 µg/gm).

Three way ANOVA represents significant association at P<0.01 level between concentration and parameters and exposure and parameters. This represents the high significant in metal accumulation but other factors are also related, but at significant level (P>0.05) Two way ANOVA represents concentrations and exposure duration are significant at 0.01 level (Table-4) and Dunet's test also reveals that the concentrations are significantly differ with control.

Sewage containing heavy metals poses multiple hazards (Berti and Cunningham, 2000) to aquatic flora and fauna. Aquatic plants have capability to accumulate heavy metals of from the media and thereby, cleaning the environment (Kara,2003; Singh *et, al.,* 2005). The data reveals that the order of accumulation of heavy metals from the sewage is as follows:

$$Fe > Cd > Pb > Zn > Ni > Cu > Mn$$

The similar observations were made in *Lemna minor* and *Phragmites karka*, was high at lower concentration of waste water and absorption capacity of the plant is marginal at subsequent concentrations and exposure duration (Pandey and Pandey, 2006; Phetsombat *et, al.,* 2006). It is evident from the present investigation that the accumulation of metals was maximum at 4 days exposure and later it was marginal, Thus, *Spirodela polyrhiza* is found to be a suitable candidate for toxicity evaluation and is used for the remediation of heavy metals from the aquatic ecosystem and environmental cleaning.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Degree College, Jamkhandi (India), Research and Development Centre, Bharthiar University, Coimbatore (Tamil Nadu), Dept.of Botany, Karnataka University Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also greateful to authors/editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed.

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CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 07 (A), pp. 39115-39120, July, 2020

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

BIOACCUMULATION OF XENOBIOTICS FROM SEWAGE BY AQUATIC MACROPHYTE

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1107.5444

ARTICLE INFO

Article History:

Received 06th April, 2020
Received in revised form 14th May, 2020
Accepted 23rd June, 2020
Published online 28th July, 2020

Key Words:

Heavy metals, accumulation, sewage, toxicity, biochemical parameters.

ABSTRACT

Increasing urbanization, industrialization, and over population and anthropogenic activities have contributed huge quantities, industrial and domestic waste water, which contains huge quantities of xenobiotics that leads to undesirable changes of the environment.

The *xenobiotics* disrupts the food chain and some toxicants are lethal even a lower concentrations. The prevailing purification technologies used for the removal of contaminants from the sewage are not only costly but causes negative impact on ecosystem subsequently .The aquatic plants have the potentiality to accumulate xenobiotics, as they were tolerant and able to withstand the pollution stress. They serve as a tool for the remediation of xenobiotics from the aquatic ecosystem. Phytoremediation is an emerging "Green Bioengineering Technology" and this concept is cheaper and alternative that hardly cost civil engineering works for environmental reconstructions. The present investigation focuses on the morphological, biochemical toxicity and accumulation profile of heavy metals in *Spirodela polyrhiza* to various concentrations of sewage i.e 25, 50, 75 and 100% at regular intervals of 4 days upto 12 days. *Spirodela* showed visible symptoms like chlorosis, stunted growth, withering of roots and lower surface of leaf turns pink to whitish. However, the test plant shows luxurious growth at 25% of sewage. Biochemical estimations like total chlorophyll, protein and carbohydrate of the test plant shows luxurious growth at 25% sewage but biochemical activity decreased with increased concentrations of sewage and exposure durations, The accumulation profile of heavy metals is directly proportional to sewage concentration and exposure duration. It was observed that the accumulation potentiality in the test plant was maximum at 4 days exposure irrespective of concentrations, however, it remains marginal at remaining exposure duration.

INTRODUCTION

The indiscriminate disposal of industrial, municipal and agricultural wastes into the aquatic ecosystem are mainly responsible for environmental pollution, which contains excess amount of organic, inorganic material and forms sources of plant nutrients, in addition to the presence of variable amount of heavy metals (Brar *et, al;* 2000 and Bajguz 2011). The response of organisms depends on their inherent sensitivity of xenobiotics, Sensitive species fails to withstand the stress. The tolerant plant species survive, thrive well and multiply in polluted environment and serve as an indicator species for environmental quality. Aquatic macrophytes / microphytes possess tremendous accumulating potential to reduce the level of toxic metals from the sewage (Salt, *et.al*., 1998). The aquatic plants have the ability to accumulate the heavy metals &have been employed for the treatment of waste water (Rai, *et. al*., 2003; Wong *et. al.,* 1996). The bio removal process using aquatic plants often exhibits two stage uptake process: An initial step, reversible, metal binding process (biosorption), followed by a slow, irreversible, ion sequestration step (bioaccumulation) (Wilde and Benemann, 1993). In view of this, the present investigation evaluates the morphological, biochemical responses and accumulation of heavy metals in *Spirodela polyrhiza* from the sewage.

MATERIALS AND METHODS

The sewage was collected from Srinagar pond near to Karnataka University Dharwad, (India) was slightly brown in colour having foul smell. The analysis of physico-chemical parameters of sewage were carried out by using standard methods of APHA (1998). The test plant *Spirodela polyrhiza* (L) were sampled from Srinagar pond. The stock plants were maintained under the laboratory conditions and experiments were carried out in triplicates. The young *Spirodela* –test plants-were selected and acclimatized for two weeks in 4% Hoagland solution in the experimental pond of 10 lt capacity.

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50gms of fresh test plants were introduced simultaneously into each of the experimental ponds containing 25%, 50%,75% and 100% sewage and tap water (control) respectively. The experiments were conducted under standard physical conditions in green house of the Department of Botany, BLDEA's Degree College Jamkhandi. The plants were harvested at the end of 4, 8 and 12 days exposure and thoroughly washed with distilled water. The 25gm of plant material was harvested and used for the morphological observation and toxicity evaluation, for estimation of total chlorophyll, protein and carbohydrate content and also for the accumulation of heavy metals. Morphological Index Parameters (MIP) viz; root length leaf length and breadth were observed for 12 days at the interval of 4 days. Photographs of *Spirodela* treated with different concentrations of sewage were taken y using Canon's Power Shot G2 Digital camera. Fresh test plant samples were macerated in 100ml of 80% (v/v) chilled acetone by using pestle and morter. The extract was centrifused and supernatant was used for the estimation of total chlorophyll by Arnon method (1949), protein estimation by Lowary's method (1951) and carbohydrate estimation by Dubois method (1956). The heavy metal estimation of sewage was carried out by using standard method (Allen *et. al.*, 1974). The dry powder of one gram plant material one ml of sewage was digested using Gerhardt digestion unit. The digested sample was used for the estimation of heavy metals *viz,* Cadmium (Cd)-228.8nm, Lead (Pb)-217.00nm,Nickel (Ni)-232.0nm, Copper (Cu)-324.7nm; Zinc (Zn)-213.9nm, Manganese (Mn)-279.5nm and Iron (Fe)-248.3nm was done by Atomic Absorption Spectrometer(AAS)-(GBC-932 plus Australia) with air acetylene oxidising flame &metal hollow cathode lamp using their respective wavelength. Working standards [SISCOP-Chem-Bombay] were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values and ±SE from experimental data with three replicates. Data were subjected to three way ANOVA with two factor interaction to find out the significance between concentration and exposure duration, concentration and parameters and exposure duration and parameters. Further Dunet's test is also applied for multiple comparisons between control and other concentrations.

Table 1 Physico-Chemical characteristics of the sewage (Madihal)

Sl. No.	Parameters	Quantity
1	pH	8.08 ± 0.01
2	Electric Conductivity (EC)	1.28 mS ± 0.01
3	Total Dissolved Solids (TDS)	680.090 ± 5.50
4	Chloride	451.00 ± 4.48
5	Hardness	341.60 ± 3.82
6	Calcium (Ca)	95.00 ± 1.94
7	Magnesium (Mg)	73.00 ± 1.20
8	Dissolved Oxygen (DO)	3.60 ± 0.24
9	Sodium (Na)	141.00 ± 2.62
10	Potassium (K)	71.00 ± 1.0
11	Chemical Oxygen Demand (COD)	298.00 ± 3.72
12	Phosphates (PO_4)	2.11 ± 0.04
13	Sulphates ($S0_4$)	102.00 ± 4.92
14	Bicarbonates (HCO_3)	552.50 ± 4.84
15	Zinc (Zn)	498.00 ±4.00
16	Copper (Cu)	210.00 ± 5.3
17	Manganese (Mg)	443.00 ± 2.10
18	Iron (Fe)	1608.00 ± 5.02
19	Cadmium (Cd)	121.00 ± 1.04
20	Lead (Pb)	2103.00 ± 3.18
21	Nickel (Ni)	371.00 ± 1.42

Sl.No. 3 to 14 – values are expressed in mg/l
Sl.No. 15 to 21 – values are expressed in µg/l
mS – milli Siemens
Mean values ± SE

Table 2 Effect of sewage on morphology of *Spirodela polyrhiza*

Sewage Concentration (%)	Exposure duration								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	1.90 ± 0.047	1.866 ± 0.054	1.866 ± 0.072	0.633 ± 0.027	0.466 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.666 ± 0.027	0.533 ± 0.108
25	2.10 ± 0.124	2.70 ± 0.124	2.80 ± 0.047	0.833 ± 0.027	0.60 ± 0.047	0.866 ± 0.027	0. 26 ± 0.047	0.90 ± zero	0.733 ± 0.272
50	2.033 ± 0.054	2.433 ± 0.190	2.466 ± 0.118	0.733 ± 0.027	0.533 ± 0.072	0.733 ± 0.027	0.6 ± 0.0	7.666 ± 0.027	0.6 ± 0.047
75	1.933 ± 0.054	1.80 ± 0.047	1.40 ± 0.047	0.60 ± 0	0.047 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.533 ± 0.072	0.466 ± 0.027
100	1.866 ± 0.054	1.733 ± 0.054	1.266 ± 0.054	0.533 ± 0.272	0.5 ± 0.047	0.466 ± 0.027	0.43 ± 0.02	0.333 ± 0.027	0.3 ± 0.047

Values are expressed in cms
Mean values ± Standard Error

Table 3 Three way ANOVA with two factor interaction for the effect of sewage on biochemical constituents of *Spirodela polyrhiza*

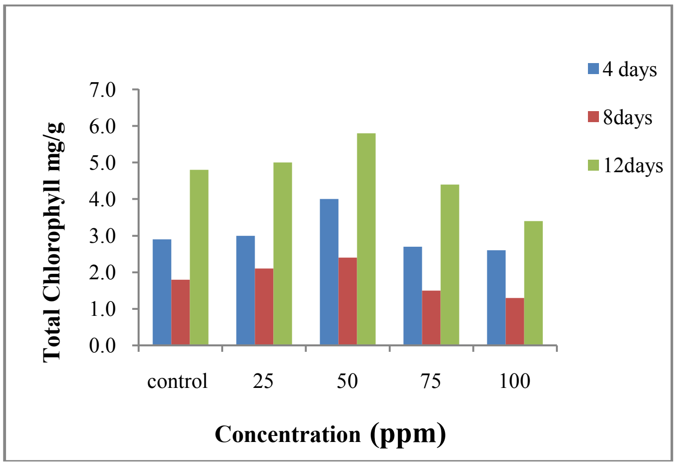
Sources of variation	Df	Sum of squares (SS)	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	8	42.282	5.285	1.187	0.365
Between concentration and parameters	8	193.221	24.153	5.425	0.002*
Between exposure and parameters	4	20.151	5.038	1.132	0.377

**Significant at $p < 0.01$ level

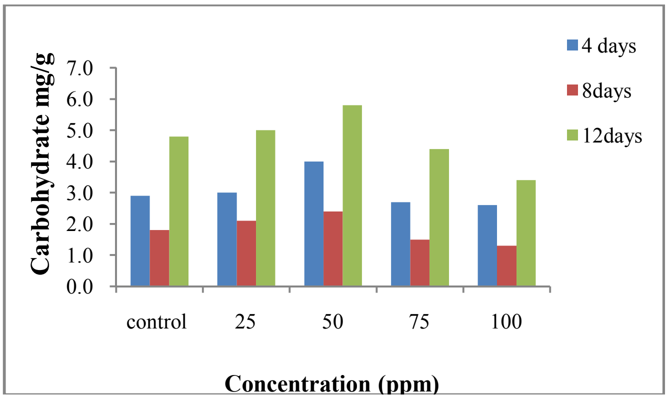
Table 4 Three way ANOVA with two factor interaction for the accumulation of heavy metals from the sewage by *Spirodela polyrhiza*

Sources of variation	Sum of squares (SS)	Df	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	532.75	8	66.594	1.99	0.068
Between concentration and parameters	132334.1	24	5513.92	165.04	0.00**
Between exposure and parameters	8507.13	12	708.92	21.21	0.000**

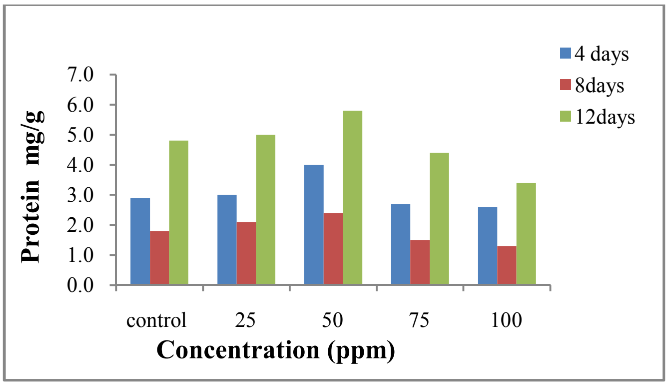
Significant at $p > 0.01$ level



A

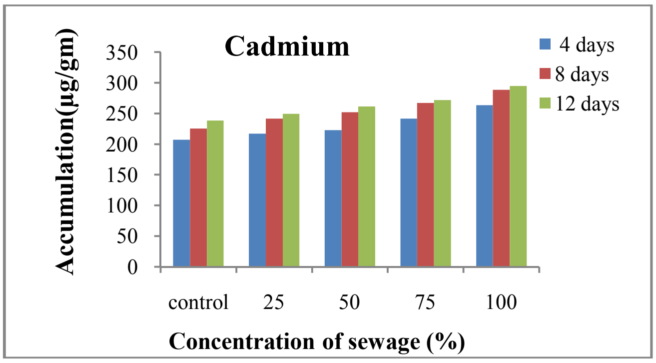


B

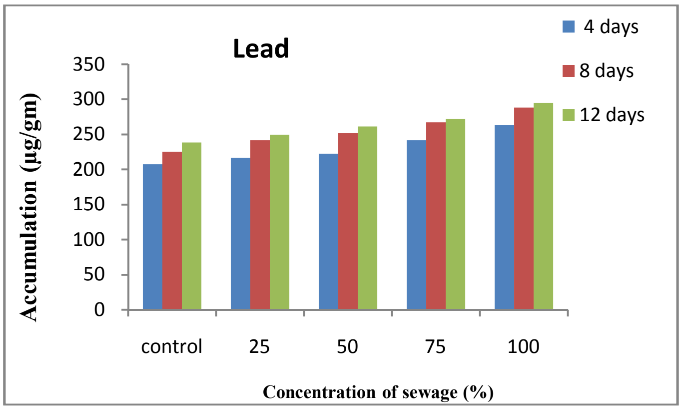


C

Fig 1 Biochemical effects of sewage on *Spirodela polyrhiza*
A) Total Chlorophyll B) Carbohydrate
B) Protein
C)



A



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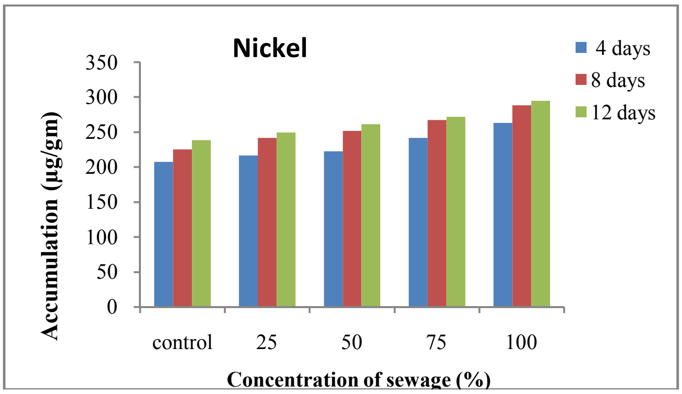
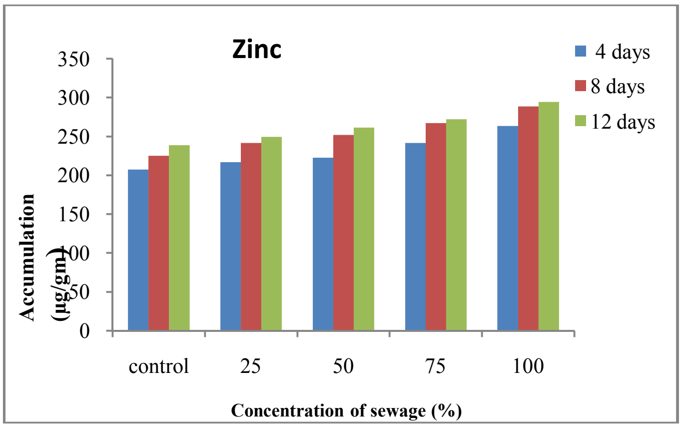
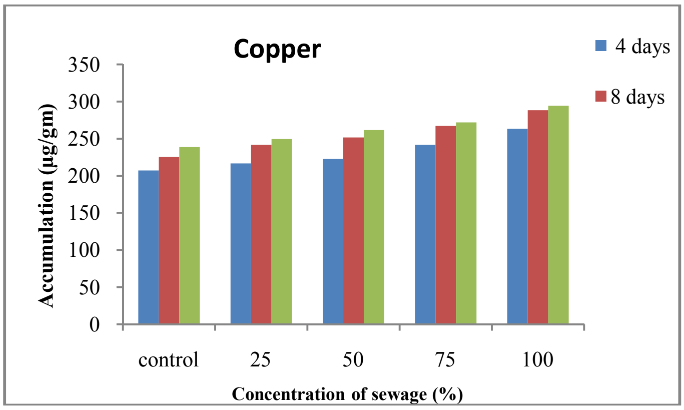


C)

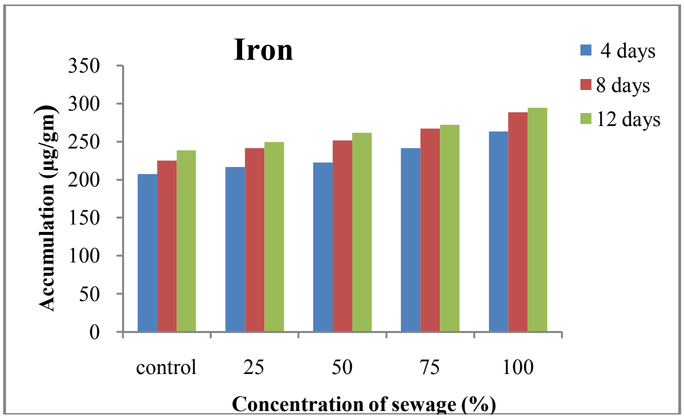


D)

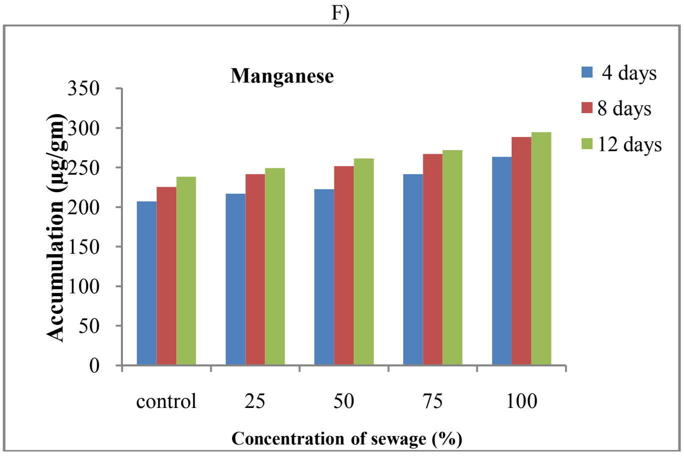
Fig 2 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*
A) Cadmium B) Lead C) Nickel D) Zinc



E)



F)



G)

Fig 3 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*
E) Copper F) Iron G) Manganese

RESULTS AND DISCUSSION

The results of physico-chemical and heavy metal analysis of sewage are present in Table -1.The sewage is slightly brown in colour with foul smell.

Toxicity Effect of Sewage Morphology

Morphometric assay is one of the quantitative tool for the assessments present in the sewage was measured by using Morphological Index Parameters (MIP). The test plant showed luxuriant growth in the laminal length and breadth at 25% sewage and it was found to promote the laminal length by 0.833 ± 0.027 cm, 0.90 ± zero cm at 4 and 12 days exposure duration and breadth by 0.60 ± 0.047 cm, 0.733 ± 0.272 cm, similarly root length by 2.10 ± 0.124 cm, 2.80 ± 0.047cm at the same exposure duration. However, the 100% sewage severely inhibit the laminal length by 0.533 ± 0.272 cm and 0.333 ± 0.027cm and breadth to about 0.5 ± 0.047 cm and 0.3 ± 0.047 cm at 4 and 12 days exposure duration. Similarly root inhibition was also noticed to the extent of 1.866 ± 0.054cm and 1.266 ± 0.054 cm at the same exposure duration. (Table 2). The plants require some of the heavy metals *viz*, Zn, Cu, Ni, Mn etc as essential macro-nutrients and are very sensitive to metabolic activities at higher concentrations (Reeves and Baker 2000)

The experimental plants shows the normal and healthy growth at lower concentration of sewage (25%) The similar observations were made by Pandit *et. al.,* (1996) in the germination of seedlings growth of *Sorghum* at 25% dairy effluent, Singh *et, al.,* (2005) also showed that 25% sugar factory effluent rich in nutrients supports optimal growth of *Potomegaton pectinatus*. In present investigation the higher concentration of sewage (100%) exhibits inhibitory effects in the test plant .The *Spirodela* shows toxic symptoms such as necrosis, yellowish, white leaves, degeneration of the leaves and disappearance of roots during 12 days exposure duration. The excess accumulation of metals in different tissues of the is responsible for morphological changes due to the interference of absorbed metal ions in the metabolism (Satyakala and Jamil, 1997).The inhibition of root growth is mainly due to the direct contact of root tip meristem with heavy metals of the experimental pond. These heavy metal brings considerable change in the rate of metabolic process of cells including nucleic acid synthesis, protein synthesis etc (Nag *et, al.,* 1981).Similar observation were also made by Marawari and Sharma (2005) in *Raphanes sativus* treated with textile waste water.

Three way ANOVA with two factor interaction for the effect of sewage on the length and breadth and also root length between root exposure and concentration is significant at 1% (P>0.01).

Toxicity Effect of Sewage on Biochemical Parameters

Biochemical changes in *Spirodela* in response to sewage are presented in the fig.(1). From the data, it is evident that the total chlorophyll present in *Spirodela* decrease with an increase in the concentration of sewage. The 25%. sewage was found to promote the synthesis of chlorophyll by 0.623 ± 0.12mg/gm (27-40%) at 4 days and 0.697 ± 0.24 mg/gm at 12 days in comparison to control. However, 100% sewage was found to inhibit the chlorophyll synthesis by 0.474 ± 0.08mg/gm (3.06%) and 0.371 ± 0.12 mg/gm (46.77%) respectively during 4 and 12 days exposure duration in comparison to control. Biochemical response of aquatic macrophyte to the toxicity of different heavy metals in an expression of their quality and quantity of the biochemical constituents. The interference of the heavy metals in cellular mechanisms by altering the structure of enzymes by changing the configuration of enzyme molecule by competitive inhibition of heavy metals. This either enhances or inhibits the synthesis of biomolecules (Brar *et, al.,* 2000). In the present investigation the experimental plant grown in 25% sewage found to promote the synthesis of chlorophyll from 0.623 ± 8.12 mg/gm (27-40%) and 0.697 ± 0.24 mg/gm, (34-35%) in 4 and 12 days exposure respectively. The increase in total chlorophyll content may be due to the optimal nutrient level which favoured the chlorophyll synthesis (Bendra and Mishra, 1983). The chlorophyll stimulation is associated with formation of phytochelatins (PCs) , plays an important role in detoxification (Prasad, 2004; Sibihil *et, al.,* 2012,).

However, the higher concentration of sewage was found to inhibit chlorophyll and directly proportional to the exposure. The 100% sewage was found to inhibit the chlorophyll in the experimental plant to about 3.06% and 46.77% at 4 and 12 days exposure respectively in comparison to control . The heavy metals present in the sewage was responsible for the degradation of photosynthetic pigments (Vajpayee *et, al.,* 2000), which ultimately causes deficiency in light harvesting capacity (Quzounidou, 1996). According to Prasad and Prasad (1987) the heavy metals are the potent inhibitors of biosynthesis of chlorophyll. The major sites of inhibition are in the formation of proteolytic phytochelatin (PC) helide reductase complex and synthesis of δ-aminolevulinic acid dehydrogenase (δ ALAD),chloroplast enzyme, which catalyses the pathway of porphobilinogen (PBG)synthesis for δ-aminolevulinic acid (ALA) (Prasad and Prasad 1987: Sing *et, al.,* 2005; Sibihi *et, al.,* 2012).

In the present investigation the 25% and 50% sewage promotes synthesis of carbohydrates. The 50% sewage promotes synthesis of carbohydrate. A remarkable carbohydrate content of 34 ± 0.12mg/gm (54.54%) was observed at 50% sewage during 12 days exposure in comparison to control. However, the carbohydrate inhibition at 100% sewage amounts to 17.02 ± 0.14mg/gm (5.55%) at 4 days and 12.0 ± 1.24mg/gm (45.45%)

at 12 days exposure duration. It was reported that the accumulation of carbohydrate in algal cells, Viz*; Anabaena* sps, *Fischerella* sps grown in highly diluted effluent and carbohydrate content is directly proportional to chlorophyll content (Renuga, 2005). The increased concentration of sewage has impact on photosynthetic activity, as the heavy metals *Viz,* Pb, Ni, Cd and Cu damages the chloroplast structure, hinders the photosynthetic assimilation (Hasan *et, al.,* 2009).

The lower concentrations of sewage , 25% and 50% found to promote the protein synthesis .The 50% sewage was also found to promote protein synthesis by 4.0 ± 0.18 mg/gm at 4 days and 5.8 ± 1.12mg/gm at an exposure duration of 12 days, however, 100% sewage was found to inhibit the protein by 2.6 ± 0.12 mg/gm at 4 days and it promotes synthesis by 3.4 ± 0.14 mg/gm during an exposure duration of 12 days. In the present investigation 25% and 50% sewage promotes the protein synthesis, but 50% more promotive by 37.93% to 41.66% at 4 and 12 days exposure in comparison to control. Similar observation was made in seedlings of *Oryza sativa* at 5% chloroalkali factory effluent (Radha and Panigrahi, 1998). The 75% and 100% sewage exhibits inhibitory effects on protein synthesis in test plant upto 8 days, however, later there will be augmentation of protein synthesis . The protein at 100% sewage is 2.8 ± 0.16 mg/g, (9.67 %), 1.8 ± 0.16 mg/g, (5.82 %) and 4.6 ± 0.12 mg/g (16.68 %) at 4, 8 and 12 days exposure. After 8 days exposure, the 100% sewage was found to augment the protein synthesis from 1.8 ± 0.16 mg/g to 4.6 ± 0.12 mg/gm was noticed due to synthesis of stress proteins or metallothionines, but later declines due to toxic effect of heavy metal on protein synthesis due to increased activity of protease, blockage of –SH group of protein. Similar observations were made by Ali *et, al., (*2003) in *Salix acomophylla* using heavy metals like Cu, Ni and Pb, it is demonstrated that the cations and anions present in the sewage affects the quality of both DNA and RNA, ultimately leads to the reduction of protein synthesis (Phalsson,1989; Marowari, *et, al.,* 2005).

Three way ANOVA with two factor interaction among the concentration, exposure duration and parameters was applied to know the association between concentration and exposure duration, concentration and parameters and exposure duration and parameters. From the data it is clear that there is (P<0.01 level) a significant association between concentration and parameters. The result reveals that the concentration and parameters are highly significant, whereas other factors are related but not significant .(Table 3).

Profile of Metal Accumulation

Spirodela showed high amelioration potential of heavy metals *Viz*, Pb, Cd, Zn, Ni, Cu,Fe and Mn etc by accumulation in its tissues (Fig 2 and 3). It is apparent from the present study that the accumulation of metals was maximum during four days exposure and thereafter marginal increase in accumulation of metals, *Spirodela* exhibit high degree of accumulation of Cd, Ni, Cu, Fe followed by Pb.At 25% sewage the *Spirodela* found to accumulate Cd to the extent of 2.00± 1.02 µg/gm and 2.75± 0.12 µg/m at 4 and 12 days exposure respectively. The phytoaccumulation is maximum (3.75±1.02 µg/m) in the plants grown in 100%. sewage during 12days exposure in comparison to control (1.75 ± 0.12 µg/m), Ni accumulation is 34.50 ± 0.12 µg/m and 44.0 ± 1.12 µg/m at 25% and 100% sewage respectively.

Iron accumulation in test plant vary 518.25 ± 1.12 µg/gm to 575.25 ± 1.12 µg/gm in 25% and 100% sewage respectively in comparison to control (258.25 ± 1.10 µg/gm) during 12 days exposure .The accumulation of Cu from the sewage 64.75 ± 0.12 µg/gm and 70.25 ± 1.10 µg/gm from 50% and 100% sewage respectively during 12 days exposure in comparison to control (52.25 ± 1.10 µg/gm). Similarly, Zn accumulation at 100% sewage is 70.25 ± 0.12 µg/gm during 12 days exposure compared to control (46.75 ± 1.12 µg/gm).

Three way ANOVA represents significant association at P<0.01 level between concentration and parameters and exposure and parameters. This represents the high significant in metal accumulation but other factors are also related, but at significant level (P>0.05) Two way ANOVA represents concentrations and exposure duration are significant at 0.01 level (Table-4) and Dunet's test also reveals that the concentrations are significantly differ with control.

Sewage containing heavy metals poses multiple hazards (Berti and Cunningham, 2000) to aquatic flora and fauna. Aquatic plants have capability to accumulate heavy metals of from the media and thereby, cleaning the environment (Kara,2003; Singh *et, al.,* 2005). The data reveals that the order of accumulation of heavy metals from the sewage is as follows:

Fe > Cd > Pb > Zn > Ni > Cu > Mn

The similar observations were made in *Lemna minor* and *Phragmites karka*, was high at lower concentration of waste water and absorption capacity of the plant is marginal at subsequent concentrations and exposure duration (Pandey and Pandey, 2006; Phetsombat *et, al.,* 2006). It is evident from the present investigation that the accumulation of metals was maximum at 4 days exposure and later it was marginal, Thus, *Spirodela polyrhiza* is found to be a suitable candidate for toxicity evaluation and is used for the remediation of heavy metals from the aquatic ecosystem and environmental cleaning.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Degree College, Jamkhandi (India), Research and Development Centre, Bharthiar University, Coimbatore (Tamil Nadu), Dept.of Botany, Karnataka University Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also greateful to authors/editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed.

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CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 07 (A), pp. 39115-39120, July, 2020

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

BIOACCUMULATION OF XENOBIOTICS FROM SEWAGE BY AQUATIC MACROPHYTE

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1107.5444

ARTICLE INFO

Article History:

Received 06th April, 2020
Received in revised form 14th May, 2020
Accepted 23rd June, 2020
Published online 28th July, 2020

Key Words:

Heavy metals, accumulation, sewage, toxicity, biochemical parameters.

ABSTRACT

Increasing urbanization, industrialization, and over population and anthropogenic activities have contributed huge quantities, industrial and domestic waste water, which contains huge quantities of xenobiotics that leads to undesirable changes of the environment.

The *xenobiotics* disrupts the food chain and some toxicants are lethal even a lower concentrations. The prevailing purification technologies used for the removal of contaminants from the sewage are not only costly but causes negative impact on ecosystem subsequently .The aquatic plants have the potentiality to accumulate xenobiotics, as they were tolerant and able to withstand the pollution stress. They serve as a tool for the remediation of xenobiotics from the aquatic ecosystem. Phytoremediation is an emerging "Green Bioengineering Technology" and this concept is cheaper and alternative that hardly cost civil engineering works for environmental reconstructions. The present investigation focuses on the morphological, biochemical toxicity and accumulation profile of heavy metals in *Spirodela polyrhiza* to various concentrations of sewage i.e 25, 50, 75 and 100% at regular intervals of 4 days upto 12 days. *Spirodela* showed visible symptoms like chlorosis, stunted growth, withering of roots and lower surface of leaf turns pink to whitish. However, the test plant shows luxurious growth at 25% of sewage. Biochemical estimations like total chlorophyll, protein and carbohydrate of the test plant shows luxurious growth at 25% sewage but biochemical activity decreased with increased concentrations of sewage and exposure durations, The accumulation profile of heavy metals is directly proportional to sewage concentration and exposure duration. It was observed that the accumulation potentiality in the test plant was maximum at 4 days exposure irrespective of concentrations, however, it remains marginal at remaining exposure duration.

INTRODUCTION

The indiscriminate disposal of industrial, municipal and agricultural wastes into the aquatic ecosystem are mainly responsible for environmental pollution, which contains excess amount of organic, inorganic material and forms sources of plant nutrients, in addition to the presence of variable amount of heavy metals (Brar *et, al;* 2000 and Bajguz 2011). The response of organisms depends on their inherent sensitivity of xenobiotics, Sensitive species fails to withstand the stress. The tolerant plant species survive, thrive well and multiply in polluted environment and serve as an indicator species for environmental quality. Aquatic macrophytes / microphytes possess tremendous accumulating potential to reduce the level of toxic metals from the sewage (Salt, *et.al*., 1998). The aquatic plants have the ability to accumulate the heavy metals &have been employed for the treatment of waste water (Rai, *et. al*., 2003; Wong *et. al.,* 1996). The bio removal process using aquatic plants often exhibits two stage uptake process: An initial step, reversible, metal binding process (biosorption), followed by a slow, irreversible, ion sequestration step (bioaccumulation) (Wilde and Benemann, 1993). In view of this, the present investigation evaluates the morphological, biochemical responses and accumulation of heavy metals in *Spirodela polyrhiza* from the sewage.

MATERIALS AND METHODS

The sewage was collected from Srinagar pond near to Karnataka University Dharwad, (India) was slightly brown in colour having foul smell. The analysis of physico-chemical parameters of sewage were carried out by using standard methods of APHA (1998). The test plant *Spirodela polyrhiza* (L) were sampled from Srinagar pond. The stock plants were maintained under the laboratory conditions and experiments were carried out in triplicates. The young *Spirodela* –test plants-were selected and acclimatized for two weeks in 4% Hoagland solution in the experimental pond of 10 lt capacity.

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50gms of fresh test plants were introduced simultaneously into each of the experimental ponds containing 25%, 50%,75% and 100% sewage and tap water (control) respectively. The experiments were conducted under standard physical conditions in green house of the Department of Botany, BLDEA's Degree College Jamkhandi. The plants were harvested at the end of 4, 8 and 12 days exposure and thoroughly washed with distilled water. The 25gm of plant material was harvested and used for the morphological observation and toxicity evaluation, for estimation of total chlorophyll, protein and carbohydrate content and also for the accumulation of heavy metals. Morphological Index Parameters (MIP) viz; root length leaf length and breadth were observed for 12 days at the interval of 4 days. Photographs of *Spirodela* treated with different concentrations of sewage were taken y using Canon's Power Shot G2 Digital camera. Fresh test plant samples were macerated in 100ml of 80% (v/v) chilled acetone by using pestle and morter. The extract was centrifused and supernatant was used for the estimation of total chlorophyll by Arnon method (1949), protein estimation by Lowary's method (1951) and carbohydrate estimation by Dubois method (1956). The heavy metal estimation of sewage was carried out by using standard method (Allen *et. al.*, 1974). The dry powder of one gram plant material one ml of sewage was digested using Gerhardt digestion unit. The digested sample was used for the estimation of heavy metals *viz,* Cadmium (Cd)-228.8nm, Lead (Pb)-217.00nm,Nickel (Ni)-232.0nm, Copper (Cu)-324.7nm; Zinc (Zn)-213.9nm, Manganese (Mn)-279.5nm and Iron (Fe)-248.3nm was done by Atomic Absorption Spectrometer(AAS)-(GBC-932 plus Australia) with air acetylene oxidising flame &metal hollow cathode lamp using their respective wavelength. Working standards [SISCOP-Chem-Bombay] were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values and ±SE from experimental data with three replicates. Data were subjected to three way ANOVA with two factor interaction to find out the significance between concentration and exposure duration, concentration and parameters and exposure duration and parameters. Further Dunet's test is also applied for multiple comparisons between control and other concentrations.

Table 1 Physico-Chemical characteristics of the sewage (Madihal)

Sl. No.	Parameters	Quantity
1	pH	8.08 ± 0.01
2	Electric Conductivity (EC)	1.28 mS ± 0.01
3	Total Dissolved Solids (TDS)	680.090 ± 5.50
4	Chloride	451.00 ± 4.48
5	Hardness	341.60 ± 3.82
6	Calcium (Ca)	95.00 ± 1.94
7	Magnesium (Mg)	73.00 ± 1.20
8	Dissolved Oxygen (DO)	3.60 ± 0.24
9	Sodium (Na)	141.00 ± 2.62
10	Potassium (K)	71.00 ± 1.0
11	Chemical Oxygen Demand (COD)	298.00 ± 3.72
12	Phosphates (PO_4)	2.11 ± 0.04
13	Sulphates ($S0_4$)	102.00 ± 4.92
14	Bicarbonates (HCO_3)	552.50 ± 4.84
15	Zinc (Zn)	498.00 ±4.00
16	Copper (Cu)	210.00 ± 5.3
17	Manganese (Mg)	443.00 ± 2.10
18	Iron (Fe)	1608.00 ± 5.02
19	Cadmium (Cd)	121.00 ± 1.04
20	Lead (Pb)	2103.00 ± 3.18
21	Nickel (Ni)	371.00 ± 1.42

Sl.No. 3 to 14 – values are expressed in mg/l
Sl.No. 15 to 21 – values are expressed in µg/l
mS – milli Siemens
Mean values ± SE

Table 2 Effect of sewage on morphology of *Spirodela polyrhiza*

Sewage Concentration (%)	Exposure duration								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	1.90 ± 0.047	1.866 ± 0.054	1.866 ± 0.072	0.633 ± 0.027	0.466 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.666 ± 0.027	0.533 ± 0.108
25	2.10 ± 0.124	2.70 ± 0.124	2.80 ± 0.047	0.833 ± 0.027	0.60 ± 0.047	0.866 ± 0.027	0. 26 ± 0.047	0.90 ± zero	0.733 ± 0.272
50	2.033 ± 0.054	2.433 ± 0.190	2.466 ± 0.118	0.733 ± 0.027	0.533 ± 0.072	0.733 ± 0.027	0.6 ± 0.0	7.666 ± 0.027	0.6 ± 0.047
75	1.933 ± 0.054	1.80 ± 0.047	1.40 ± 0.047	0.60 ± 0	0.047 ± 0.027	0.633 ± 0.027	0.5 ± 0.047	0.533 ± 0.072	0.466 ± 0.027
100	1.866 ± 0.054	1.733 ± 0.054	1.266 ± 0.054	0.533 ± 0.272	0.5 ± 0.047	0.466 ± 0.027	0.43 ± 0.02	0.333 ± 0.027	0.3 ± 0.047

Values are expressed in cms
Mean values ± Standard Error

Table 3 Three way ANOVA with two factor interaction for the effect of sewage on biochemical constituents of *Spirodela polyrhiza*

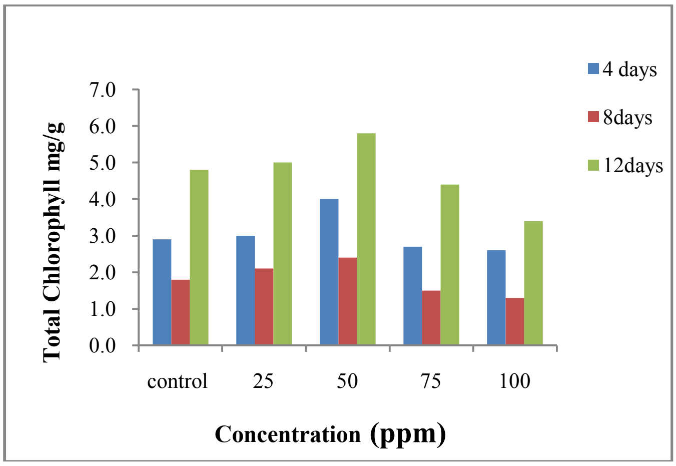
Sources of variation	Df	Sum of squares (SS)	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	8	42.282	5.285	1.187	0.365
Between concentration and parameters	8	193.221	24.153	5.425	0.002*
Between exposure and parameters	4	20.151	5.038	1.132	0.377

**Significant at $p < 0.01$ level

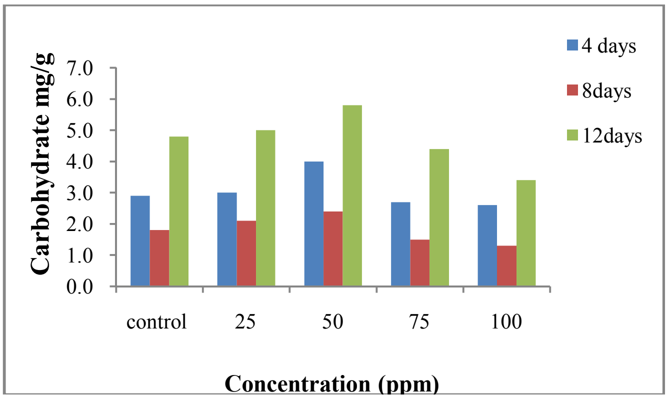
Table 4 Three way ANOVA with two factor interaction for the accumulation of heavy metals from the sewage by *Spirodela polyrhiza*

Sources of variation	Sum of squares (SS)	Df	Mean square (MS)	F	Significant (P-value)
Between concentration and exposure	532.75	8	66.594	1.99	0.068
Between concentration and parameters	132334.1	24	5513.92	165.04	0.00**
Between exposure and parameters	8507.13	12	708.92	21.21	0.000**

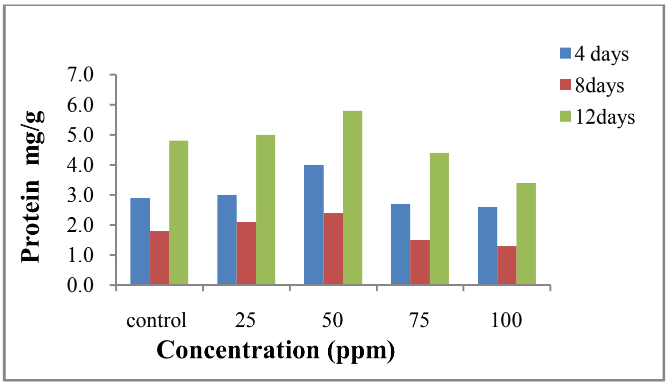
Significant at $p > 0.01$ level



A



B



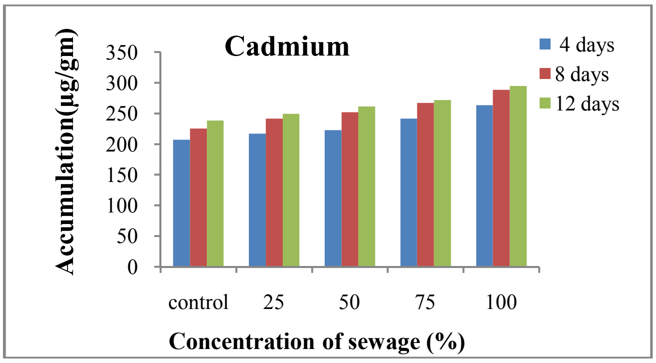
C

Fig 1 Biochemical effects of sewage on *Spirodela polyrhiza*

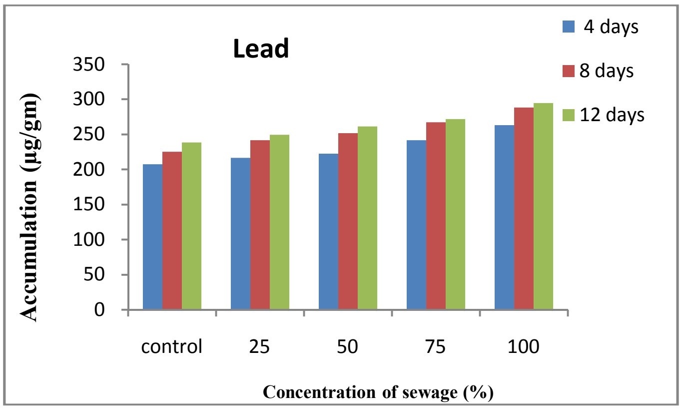
A) Total Chlorophyll B) Carbohydrate

B) Protein

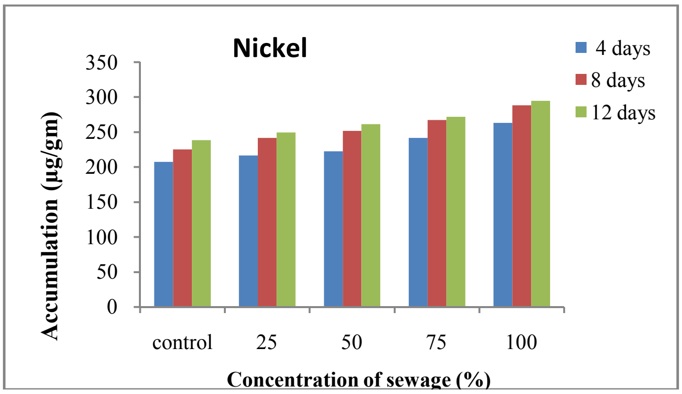
C)



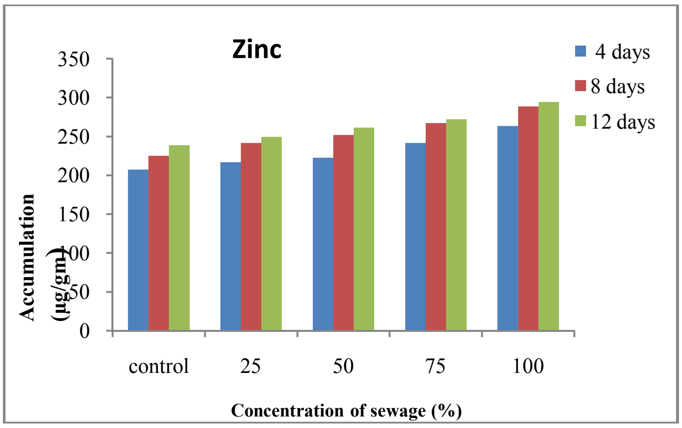
A



B



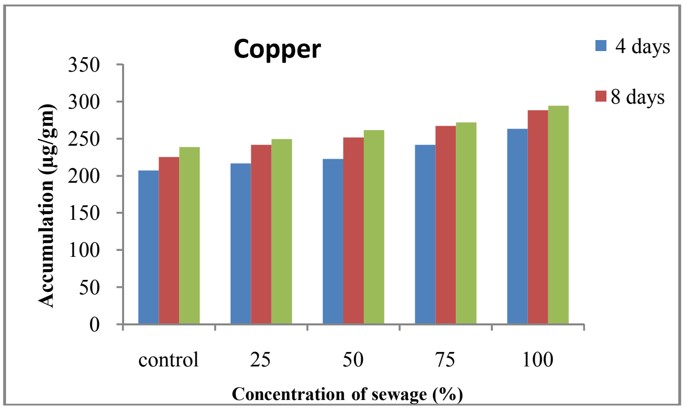
C)



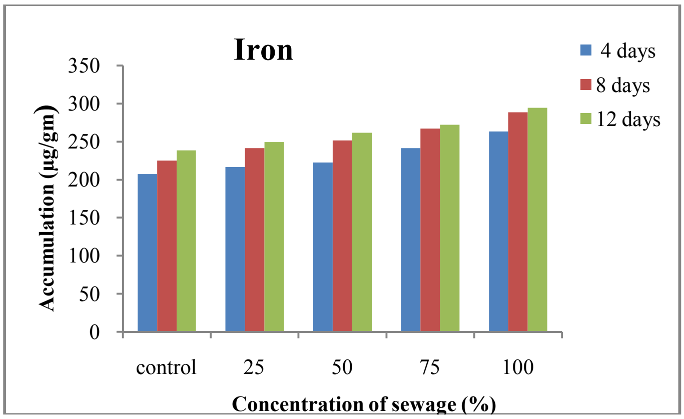
D)

Fig 2 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*

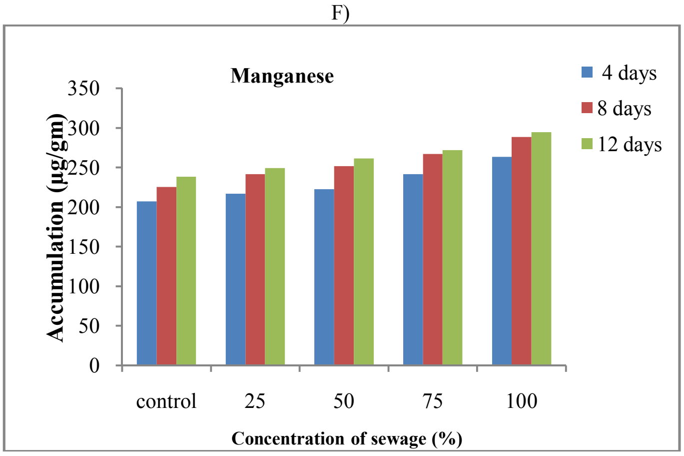
A) Cadmium B) Lead C) Nickel D) Zinc



E)



F)



G)

Fig 3 Accumulation of heavy metals from sewage by *Spirodela polyrhiza*
E) Copper F) Iron G) Manganese

RESULTS AND DISCUSSION

The results of physico-chemical and heavy metal analysis of sewage are present in Table -1.The sewage is slightly brown in colour with foul smell.

Toxicity Effect of Sewage Morphology

Morphometric assay is one of the quantitative tool for the assessments present in the sewage was measured by using Morphological Index Parameters (MIP). The test plant showed luxuriant growth in the laminal length and breadth at 25% sewage and it was found to promote the laminal length by 0.833 ± 0.027 cm, 0.90 ± zero cm at 4 and 12 days exposure duration and breadth by 0.60 ± 0.047 cm, 0.733 ± 0.272 cm, similarly root length by 2.10 ± 0.124 cm, 2.80 ± 0.047cm at the same exposure duration. However, the 100% sewage severely inhibit the laminal length by 0.533 ± 0.272 cm and 0.333 ± 0.027cm and breadth to about 0.5 ± 0.047 cm and 0.3 ± 0.047 cm at 4 and 12 days exposure duration. Similarly root inhibition was also noticed to the extent of 1.866 ± 0.054cm and 1.266 ± 0.054 cm at the same exposure duration. (Table 2). The plants require some of the heavy metals *viz*, Zn, Cu, Ni, Mn etc as essential macro-nutrients and are very sensitive to metabolic activities at higher concentrations (Reeves and Baker 2000)

The experimental plants shows the normal and healthy growth at lower concentration of sewage (25%) The similar observations were made by Pandit *et. al.,* (1996) in the germination of seedlings growth of *Sorghum* at 25% dairy effluent, Singh *et, al.,* (2005) also showed that 25% sugar factory effluent rich in nutrients supports optimal growth of *Potomegaton pectinatus*. In present investigation the higher concentration of sewage (100%) exhibits inhibitory effects in the test plant .The *Spirodela* shows toxic symptoms such as necrosis, yellowish, white leaves, degeneration of the leaves and disappearance of roots during 12 days exposure duration. The excess accumulation of metals in different tissues of the is responsible for morphological changes due to the interference of absorbed metal ions in the metabolism (Satyakala and Jamil, 1997).The inhibition of root growth is mainly due to the direct contact of root tip meristem with heavy metals of the experimental pond. These heavy metal brings considerable change in the rate of metabolic process of cells including nucleic acid synthesis, protein synthesis etc (Nag *et, al.,* 1981).Similar observation were also made by Marawari and Sharma (2005) in *Raphanes sativus* treated with textile waste water.

Three way ANOVA with two factor interaction for the effect of sewage on the length and breadth and also root length between root exposure and concentration is significant at 1% (P>0.01).

Toxicity Effect of Sewage on Biochemical Parameters

Biochemical changes in *Spirodela* in response to sewage are presented in the fig.(1). From the data, it is evident that the total chlorophyll present in *Spirodela* decrease with an increase in the concentration of sewage. The 25%. sewage was found to promote the synthesis of chlorophyll by 0.623 ± 0.12mg/gm (27-40%) at 4 days and 0.697 ± 0.24 mg/gm at 12 days in comparison to control. However, 100% sewage was found to inhibit the chlorophyll synthesis by 0.474 ± 0.08mg/gm (3.06%) and 0.371 ± 0.12 mg/gm (46.77%) respectively during 4 and 12 days exposure duration in comparison to control. Biochemical response of aquatic macrophyte to the toxicity of different heavy metals in an expression of their quality and quantity of the biochemical constituents. The interference of the heavy metals in cellular mechanisms by altering the structure of enzymes by changing the configuration of enzyme molecule by competitive inhibition of heavy metals. This either enhances or inhibits the synthesis of biomolecules (Brar *et, al.,* 2000). In the present investigation the experimental plant grown in 25% sewage found to promote the synthesis of chlorophyll from 0.623 ± 8.12 mg/gm (27-40%) and 0.697 ± 0.24 mg/gm, (34-35%) in 4 and 12 days exposure respectively. The increase in total chlorophyll content may be due to the optimal nutrient level which favoured the chlorophyll synthesis (Bendra and Mishra, 1983). The chlorophyll stimulation is associated with formation of phytochelatins (PCs) , plays an important role in detoxification (Prasad, 2004; Sibihil *et, al.,* 2012,).

However, the higher concentration of sewage was found to inhibit chlorophyll and directly proportional to the exposure. The 100% sewage was found to inhibit the chlorophyll in the experimental plant to about 3.06% and 46.77% at 4 and 12 days exposure respectively in comparison to control . The heavy metals present in the sewage was responsible for the degradation of photosynthetic pigments (Vajpayee *et, al.,* 2000), which ultimately causes deficiency in light harvesting capacity (Quzounidou, 1996). According to Prasad and Prasad (1987) the heavy metals are the potent inhibitors of biosynthesis of chlorophyll. The major sites of inhibition are in the formation of proteolytic phytochelatin (PC) helide reductase complex and synthesis of δ-aminolevulinic acid dehydrogenase (δ ALAD),chloroplast enzyme, which catalyses the pathway of porphobilinogen (PBG)synthesis for δ-aminolevulinic acid (ALA) (Prasad and Prasad 1987: Sing *et, al.,* 2005; Sibihi *et, al.,* 2012).

In the present investigation the 25% and 50% sewage promotes synthesis of carbohydrates. The 50% sewage promotes synthesis of carbohydrate. A remarkable carbohydrate content of 34 ± 0.12mg/gm (54.54%) was observed at 50% sewage during 12 days exposure in comparison to control. However, the carbohydrate inhibition at 100% sewage amounts to 17.02 ± 0.14mg/gm (5.55%) at 4 days and 12.0 ± 1.24mg/gm (45.45%)

at 12 days exposure duration. It was reported that the accumulation of carbohydrate in algal cells, Viz*; Anabaena* sps, *Fischerella* sps grown in highly diluted effluent and carbohydrate content is directly proportional to chlorophyll content (Renuga, 2005). The increased concentration of sewage has impact on photosynthetic activity, as the heavy metals *Viz,* Pb, Ni, Cd and Cu damages the chloroplast structure, hinders the photosynthetic assimilation (Hasan *et, al.,* 2009).

The lower concentrations of sewage , 25% and 50% found to promote the protein synthesis .The 50% sewage was also found to promote protein synthesis by 4.0 ± 0.18 mg/gm at 4 days and 5.8 ± 1.12mg/gm at an exposure duration of 12 days, however, 100% sewage was found to inhibit the protein by 2.6 ± 0.12 mg/gm at 4 days and it promotes synthesis by 3.4 ± 0.14 mg/gm during an exposure duration of 12 days. In the present investigation 25% and 50% sewage promotes the protein synthesis, but 50% more promotive by 37.93% to 41.66% at 4 and 12 days exposure in comparison to control. Similar observation was made in seedlings of *Oryza sativa* at 5% chloroalkali factory effluent (Radha and Panigrahi, 1998). The 75% and 100% sewage exhibits inhibitory effects on protein synthesis in test plant upto 8 days, however, later there will be augmentation of protein synthesis . The protein at 100% sewage is 2.8 ± 0.16 mg/g, (9.67 %), 1.8 ± 0.16 mg/g, (5.82 %) and 4.6 ± 0.12 mg/g (16.68 %) at 4, 8 and 12 days exposure. After 8 days exposure, the 100% sewage was found to augment the protein synthesis from 1.8 ± 0.16 mg/g to 4.6 ± 0.12 mg/gm was noticed due to synthesis of stress proteins or metallothionines, but later declines due to toxic effect of heavy metal on protein synthesis due to increased activity of protease, blockage of –SH group of protein. Similar observations were made by Ali *et, al., (*2003) in *Salix acomophylla* using heavy metals like Cu, Ni and Pb, it is demonstrated that the cations and anions present in the sewage affects the quality of both DNA and RNA, ultimately leads to the reduction of protein synthesis (Phalsson,1989; Marowari, *et, al.,* 2005).

Three way ANOVA with two factor interaction among the concentration, exposure duration and parameters was applied to know the association between concentration and exposure duration, concentration and parameters and exposure duration and parameters. From the data it is clear that there is (P<0.01 level) a significant association between concentration and parameters. The result reveals that the concentration and parameters are highly significant, whereas other factors are related but not significant .(Table 3).

Profile of Metal Accumulation

Spirodela showed high amelioration potential of heavy metals *Viz*, Pb, Cd, Zn, Ni, Cu,Fe and Mn etc by accumulation in its tissues (Fig 2 and 3). It is apparent from the present study that the accumulation of metals was maximum during four days exposure and thereafter marginal increase in accumulation of metals, *Spirodela* exhibit high degree of accumulation of Cd, Ni, Cu, Fe followed by Pb.At 25% sewage the *Spirodela* found to accumulate Cd to the extent of 2.00± 1.02 µg/gm and 2.75± 0.12 µg/m at 4 and 12 days exposure respectively. The phytoaccumulation is maximum (3.75±1.02 µg/m) in the plants grown in 100%. sewage during 12days exposure in comparison to control (1.75 ± 0.12 µg/m), Ni accumulation is 34.50 ± 0.12 µg/m and 44.0 ± 1.12 µg/m at 25% and 100% sewage respectively.

Iron accumulation in test plant vary 518.25 ± 1.12 µg/gm to 575.25 ± 1.12 µg/gm in 25% and 100% sewage respectively in comparison to control (258.25 ± 1.10 µg/gm) during 12 days exposure .The accumulation of Cu from the sewage 64.75 ± 0.12 µg/gm and 70.25 ± 1.10 µg/gm from 50% and 100% sewage respectively during 12 days exposure in comparison to control (52.25 ± 1.10 µg/gm). Similarly, Zn accumulation at 100% sewage is 70.25 ± 0.12 µg/gm during 12 days exposure compared to control (46.75 ± 1.12 µg/gm).

Three way ANOVA represents significant association at P<0.01 level between concentration and parameters and exposure and parameters. This represents the high significant in metal accumulation but other factors are also related, but at significant level (P>0.05) Two way ANOVA represents concentrations and exposure duration are significant at 0.01 level (Table-4) and Dunet's test also reveals that the concentrations are significantly differ with control.

Sewage containing heavy metals poses multiple hazards (Berti and Cunningham, 2000) to aquatic flora and fauna. Aquatic plants have capability to accumulate heavy metals of from the media and thereby, cleaning the environment (Kara,2003; Singh *et, al.,* 2005). The data reveals that the order of accumulation of heavy metals from the sewage is as follows:

Fe > Cd > Pb > Zn > Ni > Cu > Mn

The similar observations were made in *Lemna minor* and *Phragmites karka*, was high at lower concentration of waste water and absorption capacity of the plant is marginal at subsequent concentrations and exposure duration (Pandey and Pandey, 2006; Phetsombat *et, al.,* 2006). It is evident from the present investigation that the accumulation of metals was maximum at 4 days exposure and later it was marginal, Thus, *Spirodela polyrhiza* is found to be a suitable candidate for toxicity evaluation and is used for the remediation of heavy metals from the aquatic ecosystem and environmental cleaning.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Degree College, Jamkhandi (India), Research and Development Centre, Bharthiar University, Coimbatore (Tamil Nadu), Dept.of Botany, Karnataka University Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also greateful to authors/editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed.

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 08 (B), pp. 39483-39488, August, 2020

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOTOOL TO MONITOR HEAVY METAL POLLUTION IN ROADSIDE SOIL, GRASS, FICUS AND SOME ECONOMICALLY IMPORTANT CROPS

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1108.5512

ARTICLE INFO

Article History:

Received 24th May, 2020
Received in revised form 19th June, 2020
Accepted 25th July, 2020
Published online 28th August, 2020

Key Words:

Xenobiotics , Ficus, Crops, Grass, Accumulation, Bioindicators, Health

ABSTRACT

Heavy metals are important environmental pollutants and their toxicity in human, plants and animals has been received much more attention. A study was conducted to investigate the heavy metal pollution roadside soil, grass, ficus species and also some economically important crops along National highway No.4 with heavy traffic load passing along the sides from Jamkhandi to Mudhol (India). The highest levels of metal concentration of lead, cadmium, manganese, zinc, chromium and Nickel were found in the samples from very traffic congestion and were determined by using Atomic Absorption Spectrophotometer (AAS). The soil samples at a depth (0-20 cm) grass, ficus and some economically important crop leaves (wheat, maize, sugarcane) were taken from different sapling sites viz, S_1, S_2, S_3, S_4 and S_5 on state highway with high traffic road passing from Jamkhandi to Mudhol and were determined by AAS. The results showed that soil, grass, ficus and crops also contains elevated levels of metal. It was found that the primary source of the contamination occurs mainly by the vehicular exhausts. The increased circulation of toxic metals in soil, grass, ficus and crop results in the inevitable build up of xenibiotics in the food chain. The variation in heavy metal concentration is due to the changes in traffic density and anthropogenic activities . From the results it is concluded that the grass, ficus, crop plants and soil samples were used as bioindicators of metal pollution.

INTRODUCTION

Toxic level of heavy metals can cause damage to the ecology environmental nutritional and evolutionary characteristic of polluted area and consequently human residing along these areas is constantly exposed health risk (Yuan et al., 2015; Kumar et al., 2017; Zheng, 2017). Soil-plant systems to make able human productivity but suffer from pollution damage caused by human activities (Assirey and El-Shahawi, 2015; Rolli et al., 2015; Wang et al.,2017) and with the rapid development of National ecology and the subsequently traffic pollution, negative environment effect are becoming increasing apparent especially roadside plant system soil (Seedi et al., 2009; Galal and Shehata, 2015; Yang et al., 2015). Vehicular emission considered as main source of heavy metals such as Pb, Cd, Ni, Fe and Cu (Radziemska and Fronczyk, 2015; Al-fawwaz and Al-Khazaleh, 2017). The high concentration of heavy metals in urban roadside and plant samples influenced by ecological conditions like wind, rainfall, land and traffic densities (Sheikh, et al., 2016). The level of heavy metal in soil and plant inversely related with increase of distance from road edge (Kumar and Kumar, 2017). Accumulation of heavy metals in roadside soil can alter biological activities in soil and affect the enzymatic activity of microorganisms such as urease and phosphate (Flughes et al., 1980; Kumar and Kumar, 2017). Heavy metals have complex relation with plant. Histidine, citric acid, malic acid and oxalic acid present in the plant form complexes with heavy metals and convert the metals into nontoxic form (McGrah, 1994; Agarwal et al., 2007). Consumption of such contaminated crops may pose a health risk to human beings as metals form complexes with -COOH, -NH2, -SH, > NH groups present in protein to catalyse the function of enzyme (Kumar and Kumar, 2017). The new biological complexes thus formed lose their function which result in breakdown and even damage to cell also (Pirsaheb et al., 2013; Kumar and Kumar, 2017). Due to non-biodegradable and persistent nature of heavy metal, they easily accumulated in soft tissue of human being and can cause disturbance of biological process and can cause cardiovascular, kidney, liver and bone diseases (Momodu and Anyakosa, 2010; Kumar and Kumar, 2015). Information on accumulation of heavy metal on roadside soil of this study area is due to highway traffic and vehicles (Pirsaheb et al., 2013). This could be a new threat for

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agriculture. Determination of heavy metal accumulation in roadside soil , plant leaves and crop leaves may be the index of the environmental pollution of Mudhol and Jamkhandi area . Keeping this view in mind, the research was conducted to know the heavy metal accumulation of roadside soil, grass, ficus and economically important crops of the roadside and also their effect on health of the organisms.

MATERIALS AND METHODS

Jamkhandi is the city of Northern region of Karnataka at longitude 1630′ 6″ N and latitude -7516′ 17″. The city high between Jamkhandi to Mudhol is suffering from high traffic density caused by the vehicles. The grass, ficus, crop plant viz, maize, sugarcane, wheat and soil were collected, which were three meters away from the state highway (Fig. Table. 1). Grass, ficus and samples were collected from each state at three random spots that were spaced approximately at one interval. Similarly three crop plant leaves are taken at 5m, 25m, 50m and 1000m away from the grass, ficus site in triplicate. The leaves were clipped with stainless steel scissors.

The leaves of grass (*Cyanodon dactylon* L.), Ficus (*Ficus bengalensis* L.) and crops viz., Wheat (*Triticum sativum* L.), Maize (*Zea mays* L.) and Sugarcane (*Saccharum officinarum* L.) samples were dried at 80^0C for 48 hrs and was powdered and sieved through 0.2 mm sieve one gram of each sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method (mixed acid digestion method). The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made up to 100 ml. Similarly soil samples were dried, powdered and sieved through 0.2 mm sieve one gram of sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method. The resulting extract were diluted and filtered through Whattman No 41 paper and was made up to 100 ml using double distilled water and analyzed for heavy metals viz, Lead (Pb, 217.0nm), Cadmium (Cd, 228.8 nm), Copper (Cu, 324.7nm), Zinc (Zn, 213.9nm), Manganese (Mn, 279.5nm), Nickel (Ni, 232.0nm), and Chromium (Cr, 221.8 nm) filters (respective wavelengths) have been used for the estimation using Atomic Absorption Spectrophotometer (GBC 932 plus AAS, Austrelia). The working standards were prepared by serial dilution of standard stock solutions and were used for the calibration of the instrument (Pirsaheb et al., 2013).

Table 1 Description of sampling stations along the state highway of Jamkhandi to Mudhol

Sampling station		Nature of station
Control	Jamkhandi	Unpolluted area- Vehicular movement is negligible unpolluted area with less disturbance.
1	Jamkhandi bypass road	Vehicular movement is high.
2	Siddapur	Vehicular movement is high – Agricultural fields on either side of the road.
3	Prabhulingeshwar Sugar factory station	Vehicular movement is high - Agricultural fields on either side of the road but sugar factory is far away from the state highway.
4	Shirol cross	Vehicular movement is high – Agricultural fields on either side.
5	Malapur	Vehicular movement is high – Agricultural fields on either side.
6	Mudhol	Vehicular movement is high – Agricultural fields on either side & Nirani sugar factory is far away from the state highway

Table 2 Correlation coefficient of heavy metals in roadside soil and grass

S.NO	Metal	r-value
1	Lead	0.639*
2	Copper	0.478
3	Zinc	0.828*
4	Cadmium	0.748*
5	Manganese	0.531
6	Nickel	0.335
7	Chromium	0.208

Significant at **5%** level (P>0.05)
r=0.60 & above have significant correlation

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus

S.NO	**Metal**	**r-value**
1	Lead	0.641*
2	Copper	0.480
3	Zinc	0.826*
4	Cadmium	0.742*
5	Manganese	0.524
6	Nickel	0.327
7	Chromium	0.202

Significant at **5%**level(P0.05)
r=0.60 & above have significant correlation

RESULTS AND DISCUSSIONS

Pollution by heavy metals such as Pb, Cd, Ni, Cr etc is a pollution of concern (Onder and Dursun, 2006). So it has become necessary to conduct this experiment (study) to exhibit and determine the kind of environmental pollution and how far they exhibit and efficient as a bioindicator in reducing the degree of pollution in environment. The level of heavy metals in the plant and crop samples collected along the roadside (fig. 1). Correlation coefficient of heavy metals in roadside soil, grass and ficus plant samples are given in Table 2 and 3. Mean concentration of heavy metals (µg/g) and ± standard deviation in the crops is given the table 4.The ranges and arthematic mean of heavy metal concentration of soil, grass and ficus samples of state highway and control sites are presented in the table -4.

Lead is one of the major heavy metal and is considered as an environmental pollutant (Sharma and Dubey, 2005). Pb is considered as a general protoplasmic poison which accumulate and slowly acting.

The main source of Pb is exhaust fumes of automobiles, chimneys of factory, road side vehicles pollution (Eick et al., 1999). The results of our analysis show that there are significant differences for lead between sampling sites in control and polluted area. The results shows that soil tends to accumulate more Pb than grass and ficus leaves and the highest Pb level found in the roadside soil was 142.40µg/g, while the ficus, it was found that 27.38 µg/g similarly in grass it was 28.32µg/g. The mean soil Pb level of 96.74µg/g indicated considerable contamination of metal in the roadside environment, whereas, control soil has a baseline level of 72.24µg/g Pb. Much of the lead is rapidly washed on to the soil by rain water from the surface and also by the death and decomposition of the plant. The Pb deposited on soils and vegetation can also cause enhanced levels of Pb in soil microorganisms (Harrison et al., 1981; Khattak et al., 2013).

Table 4 Heavy metal accumulation profile in roadside grass, ficus and soil

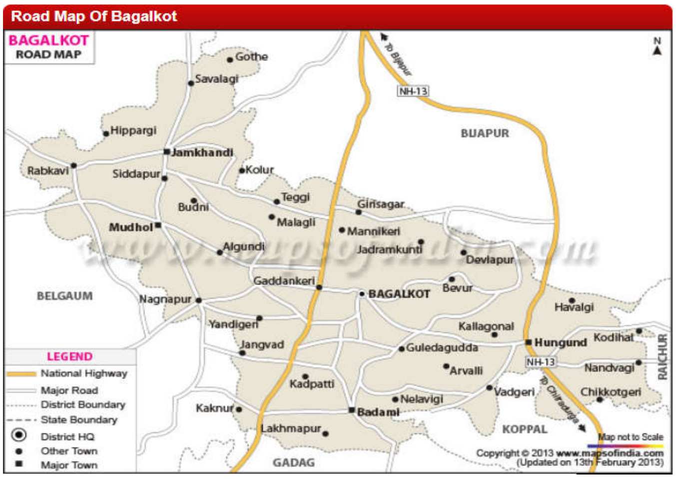
SI. NO	**Heavy metals**	**Control group µg/g (dry wt)**	**Roadside grass µg/g (dry wt)**		**Control group µg/g (dry wt)**	Roadside Ficus **µg/g (dry wt)**		**Control group µg/g (dry wt)**	**Roadside soil µg/g (dry wt)**	
			Range	**Mean± SE**	20.42	Range	**Mean± SE**		Range	Mean±**SE**
1	Lead	20.42	20.42 - 28.32	23.722 ±1.81	2.14	20.22 - 27.38	23.72 ±1.82	72.24	84.60-142.4	96.74±**8.66**
2	Copper	2.12	3.93 - 5.72	4.878 ± 0.32	15.178	3.92 - 5.72	4.70 ± 0.34	36.8	39.88-61.26	49.98±**3.3**
3	Zinc	15.173	24.48 - 34.16	32.878 ±3.11	0.88	24.42 - 36.7	30.84 ±3.10	32.0	34.26-398.02	188.8±**54.28**
4	Cadmium	0.88	1.20 - 1.78	1.594 ±0.085	16.22	1.12 - 1.78	1.42 ±0.06	2.08	1.72-2.84	2.4±**0.18**
5	Manganese	16.18	28.88 - 74.18	56.804 ±7.35	N.D	28.02 - 72.10	56.10 ±7.31	1261.42	1262.80-2034.8	1542.34±**26.59**
6	cadmium	N.D*	1.30-9.00	4.89±2.23	7.22	1.20 - 8.6	4.62 ± 2.20	124.42	129.4-962.0	326.5±**2.46**
7	Nickel	7.16	8.6 – 16.02	10.948 ±1.42		8.6 – 16.08	9.12 ± 1.42	71	74.53-118.60	88.98±**6.35**

ND* - Not detectable

Table 5 Mean concentration of heavy metals (µg/g) and ± standard deviation in crops at Shirol

Metals	**Sugarcane (Distance in mt)**				**Maize (Distance in mt)**				**Wheat (Distance in mt)**			
	5	**25**	**50**	**100**	**5**	**25**	**50**	**100**	**5**	**25**	**50**	**100**
Pb	22.72±1.81	16.42±0.02	8.12±0.02	0.08±0.02	18.21±0.03	10.21±0.02	4.26±0.02	0.08±0.01	15.72±0.02	8.21±0.02	333.27±0.07	**0.7**±0.01
Cu	4.93±0.02	4.24±0.02	3.04±0.02	2.15±0.01	4.94±0.02	4.32±0.02	3.82±0.01	2.92±0.01	4.82±0.07	4.28±0.02	3.92±0.01	2.94±0.0
Zn	32.84±0.01	20.21±0.02	22.04±0.02	14.02±0.01	30.98±0.02	24.2±0.02	16.02±0.04	12.02±0.01	31.004±0.02	22.04±0.02	18.42±0.04	12.08±0.01
Cd	1.54±0.02	1.22±0.02	1.02±0.04	0.88±0.01	1.64±0.01	1.24±0.02	0.86±0.01	0.68±0.02	1.32±0.03	1.24±0.02	0.88±0.01	0.64±0.06
Mn	56.12±0.01	38.72±0.02	28.12±0.04	15.28±0.04	52.08±0.02	46.82±0.01	36.28±0.02	18.28±0.01	53.28±0.02	41.28±0.01	32.18±0.01	16.22±0.02
Cr	4.61±0.01	4.02±0.03	3.84±0.04	1.82±0.03	4.28±0.01	3.84±0.04	2.98±0.04	1.20±0.05	4.24±0.02	3.84±0.04	2.54±0.02	1.24±0.05
Ni	4.29±0.02	2.62±0.02	0.76±0.01	0.07±0.01	2.92±0.02	1.62±0.02	0.82±0.01	0.071±0.01	2.82±0.01	1.58±0.03	0.76±0.01	0.68±0.03

Fig 1 Map showing the National Highway No. 4 passing between Jamkhandi to Mudhol



Roadside soil gave higher concentration of Cu due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of cars derived from engine wear, brussing and bearing metals (Al-Khashman, 2007). The mean Cu level in roadside soil 49.98µg/g was found to be much higher the grass 4.87µg/g and ficus 4.70µg/g.

The source of zinc in relation to automobile traffic is wearing of break lining, looses of oil and cooling liquid (Saeedi et al., 2009). Arithematic mean of Zn of the roadside soil of around Jamkhandi shows a relatively high level of 188.8µg/g with a range of 34.20µg/g -398.02µg/g. The range of Zn 24.42 µg/g – 36.7µg/g found in ficus and grass 24.48 µg/g – 34.16µg/g (roadside) is not much higher. This can be attributed to the fact that Zn as an essential element is normally in uncontaminated plants up to 100 µg/g (Ho and Tai, 1988).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process , thus, plants can easily absorbs Cd from soil and transport to the shoot system.

Cadmium induces complex changes in plants genetically, biochemical and physiological levels. Our analysis for Cd in the roadside plants and control area. Cadmium level in the roadside soil averaged about 2.4µg/g and was the lowest among the seven metals examined. The mean Cd in ficus 1.42µg/g and in grass 1.594µg/g. Our finding are in confirmation with findings of (Ho and Tai, 1988).

The soil, grass and ficus contained much higher levels of Mn than other metals examined. Roadside soil, grass and ficus had average 1542µg/g, 56.804µg/m and 56.10µg/g of Mn content of the roadside soil may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil. Chromium is considered as a serious pollutant due to wide industrial use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are determined to their growth and development. Significant differences in our analysis for Cr in soil and in plant samples are found. Chromium level too was very high in roadside soil (326.5µg/g) against the control value of 124.42µg/g. In grass it was 4.89µg/g and in ficus it was found to be 4.62µg/g against control (Zero). Nickel level was considerable and was in roadside soil (88.98 µg/g) against control value (71.0 µg/g). In grass it was 10.94µg/g and in ficus, it was found that 9.12µg/g against control (7.16µg/g).

Simple linear regression between the metals viz, Pb, Cu, Ni, Mn, Zn, Cd and Cr present in the soil, grass and ficus were calculated and are given in the Tables 3and 4.

According to simple linear regression between the metal levels in roadside soil and ficus were found in Zn, Cd and Ni are significant at 5% level ($P < 0.05$). It may be indicating the bio-

concentration of these metals in the ficus, in addition to aerial deposition. This may be attributed to the favourable root environment (Sahu and Warrier, 1985) i.e, soil conditions might have favored their absorption.

Simple linear regression in case of chromium, nickel, manganese and copper contents between the soil, grass and ficus are not significant at 5% level, were low due to low bioavailability of these metals owing to unfavorable root environment. Whatever excess content of these metals found in soil, grass and ficus was pressured to be due to aerial deposition contributed by motor vehicles and other anthropogenic activities.

The order of increment of heavy metals in roadside is as follows

Soil: Mn > Cr > Zn > Pb > Ni > Cu > Cd
Grass: Mn > Zn > Pb > Ni > Cr > Cu > Cd and
Ficus: Mn > Zn > Pb > Ni > Cu > Cr > Cd.

The elevated levels of heavy metals in the road side soil and ficus is an indication of airborne pollutants of road side environment of the urban area of Jamkhandi city and along the road soil has high retention capacity for the heavy metals (Yassoglou, et al., 1987) due to there cation exchange capacity (CFC), complexing organic substances, oxides and carbonates. Thus, contamination levels increase continuously as long as the nearby sources remain active. During the last two decades, the city of Jamkhandi to the extent has witnessed sharp increase in vehicle number due to urbanization. Similar observation in Neem and Caesalpinia in mudhurai city of southern region of Tamil Nadu (Thambavani and Vanthana, 2013) .

In soil, the lesser mobility of metals and its accumulation on a long term basis, leads to overall higher contamination level of metals, Whereas, in roadside grass, ficus represents more accumulation due to turnover of plant materials (like new growths, the senescence followed by the abscission of old parts) and meterological influence (Kabata-Pendias, 2005). Thus , the study of metal concentration of roadside soil, grass and ficus reflects the extent of aerial contamination of roadside environment. The penetration of heavy metals into the food chains due to vehicular emissions may cause a long-range ecological and health hazard.

Accumulation profile of heavy metals in Crops

There are significant differences between the distribution of heavy metals in the crops at different Sampling station with varying distances (Table. 5). The accumulation of heavy metals was found to be high in all test crops at different locations compare to control and found in the order of 5 mt > 25mt > 50mt > 1000mt (control). The mean concentration of Pb level in test sugarcane collected from 5 to 50mt from the edge of road was recorded as 22.72 ± 1.81µg/g to 8.12 ± 0.03µg/g in maize it was recorded as 18.21 ± 0.03 µg/g to 4.26 ±0.02µg/g and in wheat it was recorded as 15.72 ± 0.02 µg/g to 3.27 ± 0.07µg/g, which was significantly higher than Indian standard (2.5µg/g) recommended by Awasthi, (2000). The permissible tolerable limit in agricultural crops is 10.0 µg/g and normal is varying from 5.0 to 15.0µg/g (Kabuta-Pendias 2005).

Lead is a poisonous metal, in human it is directly absorbed in to blood stream and is stored soft tissues, bones and teeth. Due to bioaccumulation it leads to chronic damage to central nervous system (CNS) and peripheral nervous system (PNS) and also brings difficulties in pregnancy (Peokjoo et al., 2008). It includes aberrant gene transcription (Boutan et al., 2001)
The mean concentration of Cu level in test sugar cane collected from 5 to 50mt from the edge of the road was recorded as 4.93 ± 0.02 µg/g to 3.04 ± 0.02 µg/g, in maize it was recorded as 4.94 ± 0.02 µg/g to 3.82 ± 0.01 µg/g and also in wheat it was recorded 4.82 ± 0.07 µg/g to 3.92 ± 0.01 µg/g which was significantly lower than tolerable limit in agricultural crops for Cu is 50µg/g and normal limit is about 5-30µg/g (Kabuta-Pendias 2005) copper is essential element but higher concentration intake leads to severe mucosal irritation, widespread capillary damage (Salmeron and Pozo, 1989).

The tolerable limit of agricultural crops for Zinc is 300 µg/g and normal is 27-150µg/g. The mean concentration of Zinc level in sugarcane collected from 5 to 50 mt from the edge of the road was recorded as 32.81 ± 0.01µg/g to 22.04 ± 0.03 µg/g, in maize recorded as 30.98 ± 0.02µg/g to 16.02 ± 0.04µg/g and also in wheat it was 31.04 ± 0.02 µg/g to 18.42 ± 0.04 µg/g respectively.

Zinc is considered to be relatively nontoxic, however, excess amount can cause system dysfunctions that results in impairment of growth and reproduction (Dubey et al., 2007). Excess concentration of metal in the body bound in various transcription regions such as polymerase enzymes (Wang et al., 1997).

Manganese is micronutrient , essential for physiological functions. The tolerable limit for Mn in agricultural crops is 300µg/g and normal value is 30 to 300 µg/g (Kabuta-Pendias 2005). The mean concentration of Mn level in sugarcane collected from 5 to 50 mt from the edge of rod was recorded as 50.12 ± 0.01 µg/g to 28.12 ± 0.04 µg/g, in maize it was recorded as 52.08 ± 0.02 µg/g to 36.28 ± 0.02 µg/g and also in wheat it was recorded as 53.28 ± 0.02 µg/g to 32.18 ± 0.01 µg/g respectively. Mn concentrations in test crops lower than upper limit recommended by Kabuta-Pendias (2005). But higher concentration is toxic causing neuropscychiatic disorder characterized by irritability, difficulty in Walking and Speech disturbances (Singh and Kalmadhad, 2011).

The permissible tolerable limit in agricultural crops for Cd is 3.0 µg/g and normal is varying from 0.05 to 0.2 µg/g (Kabuta-Pendias 2005).In control (1000mt) crop plants maximum accumulation is recorded in sugar (0.88 ± 0.01µg/g) and minimum is 0.64 ± 0.06µg/g in wheat.

Cadmium accumulate in the human kidney, respiratory system, cardiac failure and is also associated with bone diseases (Singh and Kalamdhad-2011). (Wang and Crowley 2005) also reported that discruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of Cd-toxicity Cd level in sugar collected from 5 to 50 mt from the edge of the road was recorded as 1.54 ± 0.02 µg/g to 1.02 ± 0.04 µg/g, in maize it was recorded as 1.64 ± 0.01 µg/g to 0.86 ± 0.01µg/g and also it was recorded to about 1.32 ± 0.03 µg/g to 0.88 ± 0.04µg/g in wheat respectively.

Chromium is considered as a serious environmental pollutant, due to industrial (wide) use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are detrimental to their growth. The mean concentration of Cr level in sugarcane

collected from 5 to 50 mt from the edge of road was recorded as 4.61±0.01 µg/g to 3.84±0.04 µg/g; in maize it was recorded as 4.28 ± 0.01 µg/g to 2.98 ± 0.04 µg/g and also in wheat to about 4.24 ± 0.02 µg/g to 2.54 ± 0.02 µg/g respectively.

Nickel has been considered to be an trace essential trace element for human (Animal) health (Zhuang et al., 2012). The permissible tolerable limit in agricultural crops is 50µg/g and normal is about 0.1 to 5.0µg/g. The mean concentration of Ni level in sugarcane collected from 5 to 50 mt from the edge of road was recorded as 4.29 ± 0.02 µg/g to 0.76 ± 0.01µg/g, in maize it was 2.92 ± 0.02 µg/g to 0.82 ± 0.01 µg/g and also in wheat it was 2.82 ± 0.01 µg/g to 0.76 ± 0.01 µg/g respectively. Nickel occurs mainly in the form of Sulphide and silicate minerals. Ni when administrated to animals is rapidly distributed to kidneys, pituitary, lungs, skin, adrinals, ovaries and testis (Sundarman-1989). Ni is carcinogenic to human and risks are highest for lung and nasal cancers. Ni also damages DNA directly through reactive oxygen species (McCoy and Kinney,1992).

CONCLUSION

Based in the analysis and results, it could be concluded that study on roadside soil, test plants and crops confirmed that vehicular emission is potential source of environmental pollution. The high level concentration Lead, Cadmium and Nickel concentration in soil will affect the health of the residents as well as surrounding communities, which may also affect soil fertility too. The consumption of these crops can considered safe with no risk to human health. The average intake of metals in long time low level body accumulation of heavy metals and detrimental impact becomes apparent only several year of exposure. These findings also suggest that special attention should be taken to this traffic related environmental issue and further suggest that serious affords required to reduced the high level of soil remediation and before the consumption of crops/vegetables should washed to remove significant amount of aerial accumulation from the surface of crops/vegetables. Finally, it is recommended that economical plant (vegetable/crops) should not be cultivated along the roadside and especially in high traffic density areas.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Com.BHS Arts and TGP Science College, Jamkhandi (Karnataka), Principal, B.V.V. Snaghas, Basaveshwar Science College Bagalkot (Karnataka), Chairman, PG Department Botany, Karnataka University, Dharawad (Karnataka) for providing necessary facilities to carry out research work.

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 08 (B), pp. 39483-39488, August, 2020

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOTOOL TO MONITOR HEAVY METAL POLLUTION IN ROADSIDE SOIL, GRASS, FICUS AND SOME ECONOMICALLY IMPORTANT CROPS

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1108.5512

ARTICLE INFO

Article History:

Received 24th May, 2020
Received in revised form 19th June, 2020
Accepted 25th July, 2020
Published online 28th August, 2020

Key Words:

Xenobiotics , Ficus, Crops, Grass, Accumulation, Bioindicators, Health

ABSTRACT

Heavy metals are important environmental pollutants and their toxicity in human, plants and animals has been received much more attention. A study was conducted to investigate the heavy metal pollution roadside soil, grass, ficus species and also some economically important crops along National highway No.4 with heavy traffic load passing along the sides from Jamkhandi to Mudhol (India). The highest levels of metal concentration of lead, cadmium, manganese, zinc, chromium and Nickel were found in the samples from very traffic congestion and were determined by using Atomic Absorption Spectrophotometer (AAS). The soil samples at a depth (0-20 cm) grass, ficus and some economically important crop leaves (wheat, maize, sugarcane) were taken from different sapling sites viz, S_1, S_2, S_3, S_4 and S_5 on state highway with high traffic road passing from Jamkhandi to Mudhol and were determined by AAS. The results showed that soil, grass, ficus and crops also contains elevated levels of metal. It was found that the primary source of the contamination occurs mainly by the vehicular exhausts. The increased circulation of toxic metals in soil, grass, ficus and crop results in the inevitable build up of xenibiotics in the food chain. The variation in heavy metal concentration is due to the changes in traffic density and anthropogenic activities . From the results it is concluded that the grass, ficus, crop plants and soil samples were used as bioindicators of metal pollution.

INTRODUCTION

Toxic level of heavy metals can cause damage to the ecology environmental nutritional and evolutionary characteristic of polluted area and consequently human residing along these areas is constantly exposed health risk (Yuan et al., 2015; Kumar et al., 2017; Zheng, 2017). Soil-plant systems to make able human productivity but suffer from pollution damage caused by human activities (Assirey and El-Shahawi, 2015; Rolli et al., 2015; Wang et al.,2017) and with the rapid development of National ecology and the subsequently traffic pollution, negative environment effect are becoming increasing apparent especially roadside plant system soil (Seedi et al., 2009; Galal and Shehata, 2015; Yang et al., 2015). Vehicular emission considered as main source of heavy metals such as Pb, Cd, Ni, Fe and Cu (Radziemska and Fronczyk, 2015; Al-fawwaz and Al-Khazaleh, 2017). The high concentration of heavy metals in urban roadside and plant samples influenced by ecological conditions like wind, rainfall, land and traffic densities (Sheikh, et al., 2016). The level of heavy metal in soil and plant inversely related with increase of distance from road edge (Kumar and Kumar, 2017). Accumulation of heavy metals in roadside soil can alter biological activities in soil and affect the enzymatic activity of microorganisms such as urease and phosphate (Flughes et al., 1980; Kumar and Kumar, 2017). Heavy metals have complex relation with plant. Histidine, citric acid, malic acid and oxalic acid present in the plant form complexes with heavy metals and convert the metals into nontoxic form (McGrah, 1994; Agarwal et al., 2007). Consumption of such contaminated crops may pose a health risk to human beings as metals form complexes with -COOH, -NH2, -SH, > NH groups present in protein to catalyse the function of enzyme (Kumar and Kumar, 2017). The new biological complexes thus formed lose their function which result in breakdown and even damage to cell also (Pirsaheb et al., 2013; Kumar and Kumar, 2017). Due to non-biodegradable and persistent nature of heavy metal, they easily accumulated in soft tissue of human being and can cause disturbance of biological process and can cause cardiovascular, kidney, liver and bone diseases (Momodu and Anyakosa, 2010; Kumar and Kumar, 2015). Information on accumulation of heavy metal on roadside soil of this study area is due to highway traffic and vehicles (Pirsaheb et al., 2013). This could be a new threat for

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agriculture. Determination of heavy metal accumulation in roadside soil , plant leaves and crop leaves may be the index of the environmental pollution of Mudhol and Jamkhandi area . Keeping this view in mind, the research was conducted to know the heavy metal accumulation of roadside soil, grass, ficus and economically important crops of the roadside and also their effect on health of the organisms.

MATERIALS AND METHODS

Jamkhandi is the city of Northern region of Karnataka at longitude 1630′ 6″ N and latitude -7516′ 17″. The city high between Jamkhandi to Mudhol is suffering from high traffic density caused by the vehicles. The grass, ficus, crop plant viz, maize, sugarcane, wheat and soil were collected, which were three meters away from the state highway (Fig. Table. 1). Grass, ficus and samples were collected from each state at three random spots that were spaced approximately at one interval. Similarly three crop plant leaves are taken at 5m, 25m, 50m and 1000m away from the grass, ficus site in triplicate. The leaves were clipped with stainless steel scissors.

The leaves of grass (*Cyanodon dactylon* L.), Ficus (*Ficus bengalensis* L.) and crops viz., Wheat (*Triticum sativum* L.), Maize (*Zea mays* L.) and Sugarcane (*Saccharum officinarum* L.) samples were dried at 80^0C for 48 hrs and was powdered and sieved through 0.2 mm sieve one gram of each sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method (mixed acid digestion method). The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made up to 100 ml. Similarly soil samples were dried, powdered and sieved through 0.2 mm sieve one gram of sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method. The resulting extract were diluted and filtered through Whattman No 41 paper and was made up to 100 ml using double distilled water and analyzed for heavy metals viz, Lead (Pb, 217.0nm), Cadmium (Cd, 228.8 nm), Copper (Cu, 324.7nm), Zinc (Zn, 213.9nm), Manganese (Mn, 279.5nm), Nickel (Ni, 232.0nm), and Chromium (Cr, 221.8 nm) filters (respective wavelengths) have been used for the estimation using Atomic Absorption Spectrophotometer (GBC 932 plus AAS, Austrelia). The working standards were prepared by serial dilution of standard stock solutions and were used for the calibration of the instrument (Pirsaheb et al., 2013).

Table 1 Description of sampling stations along the state highway of Jamkhandi to Mudhol

Sampling station		Nature of station
Control	Jamkhandi	Unpolluted area- Vehicular movement is negligible unpolluted area with less disturbance.
1	Jamkhandi bypass road	Vehicular movement is high.
2	Siddapur	Vehicular movement is high – Agricultural fields on either side of the road.
3	Prabhulingeshwar Sugar factory station	Vehicular movement is high - Agricultural fields on either side of the road but sugar factory is far away from the state highway.
4	Shirol cross	Vehicular movement is high – Agricultural fields on either side.
5	Malapur	Vehicular movement is high – Agricultural fields on either side.
6	Mudhol	Vehicular movement is high – Agricultural fields on either side & Nirani sugar factory is far away from the state highway

Table 2 Correlation coefficient of heavy metals in roadside soil and grass

S.NO	Metal	r-value
1	Lead	0.639*
2	Copper	0.478
3	Zinc	0.828*
4	Cadmium	0.748*
5	Manganese	0.531
6	Nickel	0.335
7	Chromium	0.208

Significant at **5%** level (P>0.05)
r=0.60 & above have significant correlation

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus

S.NO	Metal	r-value
1	Lead	0.641*
2	Copper	0.480
3	Zinc	0.826*
4	Cadmium	0.742*
5	Manganese	0.524
6	Nickel	0.327
7	Chromium	0.202

Significant at **5%**level(P0.05)
r=0.60 & above have significant correlation

RESULTS AND DISCUSSIONS

Pollution by heavy metals such as Pb, Cd, Ni, Cr etc is a pollution of concern (Onder and Dursun, 2006). So it has become necessary to conduct this experiment (study) to exhibit and determine the kind of environmental pollution and how far they exhibit and efficient as a bioindicator in reducing the degree of pollution in environment. The level of heavy metals in the plant and crop samples collected along the roadside (fig. 1). Correlation coefficient of heavy metals in roadside soil, grass and ficus plant samples are given in Table 2 and 3. Mean concentration of heavy metals (µg/g) and ± standard deviation in the crops is given the table 4.The ranges and arthematic mean of heavy metal concentration of soil, grass and ficus samples of state highway and control sites are presented in the table -4.

Lead is one of the major heavy metal and is considered as an environmental pollutant (Sharma and Dubey, 2005). Pb is considered as a general protoplasmic poison which accumulate and slowly acting.

The main source of Pb is exhaust fumes of automobiles, chimneys of factory, road side vehicles pollution (Eick et al., 1999). The results of our analysis show that there are significant differences for lead between sampling sites in control and polluted area. The results shows that soil tends to accumulate more Pb than grass and ficus leaves and the highest Pb level found in the roadside soil was 142.40µg/g, while the ficus, it was found that 27.38 µg/g similarly in grass it was 28.32µg/g. The mean soil Pb level of 96.74µg/g indicated considerable contamination of metal in the roadside environment, whereas, control soil has a baseline level of 72.24µg/g Pb. Much of the lead is rapidly washed on to the soil by rain water from the surface and also by the death and decomposition of the plant. The Pb deposited on soils and vegetation can also cause enhanced levels of Pb in soil microorganisms (Harrison et al., 1981; Khattak et al., 2013).

Table 4 Heavy metal accumulation profile in roadside grass, ficus and soil

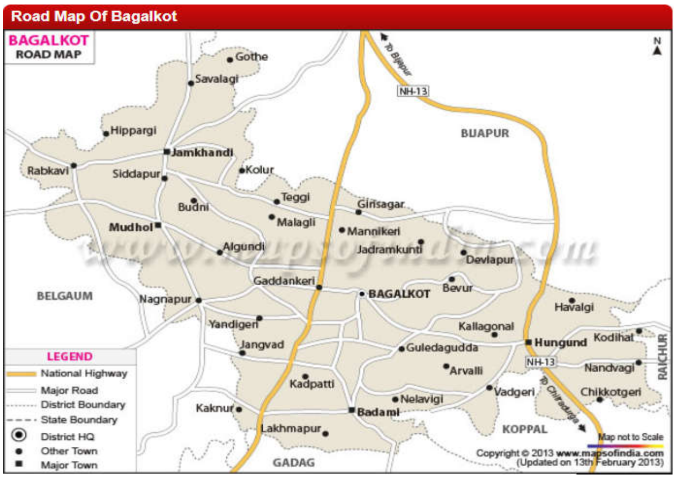
SI. NO	**Heavy metals**	**Control group µg/g (dry wt)**	**Roadside grass µg/g (dry wt)**		**Control group µg/g (dry wt)**	Roadside Ficus **µg/g (dry wt)**		**Control group µg/g (dry wt)**	**Roadside soil µg/g (dry wt)**	
			Range	**Mean± SE**	20.42	Range	**Mean± SE**		Range	Mean±**SE**
1	Lead	20.42	20.42 - 28.32	23.722 ±1.81	2.14	20.22 - 27.38	23.72 ±1.82	72.24	84.60-142.4	96.74±**8.66**
2	Copper	2.12	3.93 - 5.72	4.878 ± 0.32	15.178	3.92 - 5.72	4.70 ± 0.34	36.8	39.88-61.26	49.98±**3.3**
3	Zinc	15.173	24.48 - 34.16	32.878 ±3.11	0.88	24.42 - 36.7	30.84 ±3.10	32.0	34.26-398.02	188.8±**54.28**
4	Cadmium	0.88	1.20 - 1.78	1.594 ±0.085	16.22	1.12 - 1.78	1.42 ±0.06	2.08	1.72-2.84	2.4±**0.18**
5	Manganese	16.18	28.88 - 74.18	56.804 ±7.35	N.D	28.02 - 72.10	56.10 ±7.31	1261.42	1262.80-2034.8	1542.34±**26.59**
6	cadmium	N.D*	1.30-9.00	4.89±2.23	7.22	1.20 - 8.6	4.62 ± 2.20	124.42	129.4-962.0	326.5±**2.46**
7	Nickel	7.16	8.6 – 16.02	10.948 ±1.42		8.6 – 16.08	9.12 ± 1.42	71	74.53-118.60	88.98±**6.35**

ND* - Not detectable

Table 5 Mean concentration of heavy metals (µg/g) and ± standard deviation in crops at Shirol

Metals	**Sugarcane (Distance in mt)**				**Maize (Distance in mt)**				**Wheat (Distance in mt)**			
	5	**25**	**50**	**100**	**5**	**25**	**50**	**100**	**5**	**25**	**50**	**100**
Pb	22.72±1.81	16.42±0.02	8.12±0.02	0.08±0.02	18.21±0.03	10.21±0.02	4.26±0.02	0.08±0.01	15.72±0.02	8.21±0.02	333.27±0.07	**0.7**±0.01
Cu	4.93±0.02	4.24±0.02	3.04±0.02	2.15±0.01	4.94±0.02	4.32±0.02	3.82±0.01	2.92±0.01	4.82±0.07	4.28±0.02	3.92±0.01	2.94±0.0
Zn	32.84±0.01	20.21±0.02	22.04±0.02	14.02±0.01	30.98±0.02	24.2±0.02	16.02±0.04	12.02±0.01	31.004±0.02	22.04±0.02	18.42±0.04	12.08±0.01
Cd	1.54±0.02	1.22±0.02	1.02±0.04	0.88±0.01	1.64±0.01	1.24±0.02	0.86±0.01	0.68±0.02	1.32±0.03	1.24±0.02	0.88±0.01	0.64±0.06
Mn	56.12±0.01	38.72±0.02	28.12±0.04	15.28±0.04	52.08±0.02	46.82±0.01	36.28±0.02	18.28±0.01	53.28±0.02	41.28±0.01	32.18±0.01	16.22±0.02
Cr	4.61±0.01	4.02±0.03	3.84±0.04	1.82±0.03	4.28±0.01	3.84±0.04	2.98±0.04	1.20±0.05	4.24±0.02	3.84±0.04	2.54±0.02	1.24±0.05
Ni	4.29±0.02	2.62±0.02	0.76±0.01	0.07±0.01	2.92±0.02	1.62±0.02	0.82±0.01	0.071±0.01	2.82±0.01	1.58±0.03	0.76±0.01	0.68±0.03

Fig 1 Map showing the National Highway No. 4 passing between Jamkhandi to Mudhol



Roadside soil gave higher concentration of Cu due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of cars derived from engine wear, brussing and bearing metals (Al-Khashman, 2007). The mean Cu level in roadside soil 49.98µg/g was found to be much higher the grass 4.87µg/g and ficus 4.70µg/g.

The source of zinc in relation to automobile traffic is wearing of break lining, looses of oil and cooling liquid (Saeedi et al., 2009). Arithematic mean of Zn of the roadside soil of around Jamkhandi shows a relatively high level of 188.8µg/g with a range of 34.20µg/g -398.02µg/g. The range of Zn 24.42 µg/g – 36.7µg/g found in ficus and grass 24.48 µg/g – 34.16µg/g (roadside) is not much higher. This can be attributed to the fact that Zn as an essential element is normally in uncontaminated plants up to 100 µg/g (Ho and Tai, 1988).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process , thus, plants can easily absorbs Cd from soil and transport to the shoot system.

Cadmium induces complex changes in plants genetically, biochemical and physiological levels. Our analysis for Cd in the roadside plants and control area. Cadmium level in the roadside soil averaged about 2.4µg/g and was the lowest among the seven metals examined. The mean Cd in ficus 1.42µg/g and in grass 1.594µg/g. Our finding are in confirmation with findings of (Ho and Tai, 1988).

The soil, grass and ficus contained much higher levels of Mn than other metals examined. Roadside soil, grass and ficus had average 1542µg/g, 56.804µg/m and 56.10µg/g of Mn content of the roadside soil may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil. Chromium is considered as a serious pollutant due to wide industrial use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are determined to their growth and development. Significant differences in our analysis for Cr in soil and in plant samples are found. Chromium level too was very high in roadside soil (326.5µg/g) against the control value of 124.42µg/g. In grass it was 4.89µg/g and in ficus it was found to be 4.62µg/g against control (Zero). Nickel level was considerable and was in roadside soil (88.98 µg/g) against control value (71.0 µg/g). In grass it was 10.94µg/g and in ficus, it was found that 9.12µg/g against control (7.16µg/g).

Simple linear regression between the metals viz, Pb, Cu, Ni, Mn, Zn, Cd and Cr present in the soil, grass and ficus were calculated and are given in the Tables 3and 4.

According to simple linear regression between the metal levels in roadside soil and ficus were found in Zn, Cd and Ni are significant at 5% level ($P < 0.05$). It may be indicating the bio-

concentration of these metals in the ficus, in addition to aerial deposition. This may be attributed to the favourable root environment (Sahu and Warrier, 1985) i.e, soil conditions might have favored their absorption.

Simple linear regression in case of chromium, nickel, manganese and copper contents between the soil, grass and ficus are not significant at 5% level, were low due to low bioavailability of these metals owing to unfavorable root environment. Whatever excess content of these metals found in soil, grass and ficus was pressured to be due to aerial deposition contributed by motor vehicles and other anthropogenic activities.

The order of increment of heavy metals in roadside is as follows

Soil: Mn > Cr > Zn > Pb > Ni > Cu > Cd
Grass: Mn > Zn > Pb > Ni > Cr > Cu > Cd and
Ficus: Mn > Zn > Pb > Ni > Cu > Cr > Cd.

The elevated levels of heavy metals in the road side soil and ficus is an indication of airborne pollutants of road side environment of the urban area of Jamkhandi city and along the road soil has high retention capacity for the heavy metals (Yassoglou, et al., 1987) due to there cation exchange capacity (CFC), complexing organic substances, oxides and carbonates. Thus, contamination levels increase continuously as long as the nearby sources remain active. During the last two decades, the city of Jamkhandi to the extent has witnessed sharp increase in vehicle number due to urbanization. Similar observation in Neem and Caesalpinia in mudhurai city of southern region of Tamil Nadu (Thambavani and Vanthana, 2013) .
In soil, the lesser mobility of metals and its accumulation on a long term basis, leads to overall higher contamination level of metals, Whereas, in roadside grass, ficus represents more accumulation due to turnover of plant materials (like new growths, the senescence followed by the abscission of old parts) and meterological influence (Kabata-Pendias, 2005). Thus , the study of metal concentration of roadside soil, grass and ficus reflects the extent of aerial contamination of roadside environment. The penetration of heavy metals into the food chains due to vehicular emissions may cause a long-range ecological and health hazard.

Accumulation profile of heavy metals in Crops

There are significant differences between the distribution of heavy metals in the crops at different Sampling station with varying distances (Table. 5). The accumulation of heavy metals was found to be high in all test crops at different locations compare to control and found in the order of 5 mt > 25mt > 50mt > 1000mt (control). The mean concentration of Pb level in test sugarcane collected from 5 to 50mt from the edge of road was recorded as 22.72 ± 1.81µg/g to 8.12 ± 0.03µg/g in maize it was recorded as 18.21 ± 0.03 µg/g to 4.26 ±0.02µg/g and in wheat it was recorded as 15.72 ± 0.02 µg/g to 3.27 ± 0.07µg/g, which was significantly higher than Indian standard (2.5µg/g) recommended by Awasthi, (2000). The permissible tolerable limit in agricultural crops is 10.0 µg/g and normal is varying from 5.0 to 15.0µg/g (Kabuta-Pendias 2005).

Lead is a poisonous metal, in human it is directly absorbed in to blood stream and is stored soft tissues, bones and teeth. Due to bioaccumulation it leads to chronic damage to central nervous system (CNS) and peripheral nervous system (PNS) and also brings difficulties in pregnancy (Peokjoo et al., 2008). It includes aberrant gene transcription (Boutan et al., 2001)
The mean concentration of Cu level in test sugar cane collected from 5 to 50mt from the edge of the road was recorded as 4.93 ± 0.02 µg/g to 3.04 ± 0.02 µg/g, in maize it was recorded as 4.94 ± 0.02 µg/g to 3.82 ± 0.01 µg/g and also in wheat it was recorded 4.82 ± 0.07 µg/g to 3.92 ± 0.01 µg/g which was significantly lower than tolerable limit in agricultural crops for Cu is 50µg/g and normal limit is about 5-30µg/g (Kabuta-Pendias 2005) copper is essential element but higher concentration intake leads to severe mucosal irritation, widespread capillary damage (Salmeron and Pozo, 1989).

The tolerable limit of agricultural crops for Zinc is 300 µg/g and normal is 27-150µg/g. The mean concentration of Zinc level in sugarcane collected from 5 to 50 mt from the edge of the road was recorded as 32.81 ± 0.01µg/g to 22.04 ± 0.03 µg/g, in maize recorded as 30.98 ± 0.02µg/g to 16.02 ± 0.04µg/g and also in wheat it was 31.04 ± 0.02 µg/g to 18.42 ± 0.04 µg/g respectively.

Zinc is considered to be relatively nontoxic, however, excess amount can cause system dysfunctions that results in impairment of growth and reproduction (Dubey et al., 2007). Excess concentration of metal in the body bound in various transcription regions such as polymerase enzymes (Wang et al., 1997).

Manganese is micronutrient , essential for physiological functions. The tolerable limit for Mn in agricultural crops is 300µg/g and normal value is 30 to 300 µg/g (Kabuta-Pendias 2005). The mean concentration of Mn level in sugarcane collected from 5 to 50 mt from the edge of rod was recorded as 50.12 ± 0.01 µg/g to 28.12 ± 0.04 µg/g, in maize it was recorded as 52.08 ± 0.02 µg/g to 36.28 ± 0.02 µg/g and also in wheat it was recorded as 53.28 ± 0.02 µg/g to 32.18 ± 0.01 µg/g respectively. Mn concentrations in test crops lower than upper limit recommended by Kabuta-Pendias (2005). But higher concentration is toxic causing neuropscychiatic disorder characterized by irritability, difficulty in Walking and Speech disturbances (Singh and Kalmadhad, 2011).

The permissible tolerable limit in agricultural crops for Cd is 3.0 µg/g and normal is varying from 0.05 to 0.2 µg/g (Kabuta-Pendias 2005).In control (1000mt) crop plants maximum accumulation is recorded in sugar (0.88 ± 0.01µg/g) and minimum is 0.64 ± 0.06µg/g in wheat.

Cadmium accumulate in the human kidney, respiratory system, cardiac failure and is also associated with bone diseases (Singh and Kalamdhad-2011). (Wang and Crowley 2005) also reported that discruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of Cd-toxicity Cd level in sugar collected from 5 to 50 mt from the edge of the road was recorded as 1.54 ± 0.02 µg/g to 1.02 ± 0.04 µg/g, in maize it was recorded as 1.64 ± 0.01 µg/g to 0.86 ± 0.01µg/g and also it was recorded to about 1.32 ± 0.03 µg/g to 0.88 ± 0.04µg/g in wheat respectively.

Chromium is considered as a serious environmental pollutant, due to industrial (wide) use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are detrimental to their growth. The mean concentration of Cr level in sugarcane

collected from 5 to 50 mt from the edge of road was recorded as 4.61±0.01 µg/g to 3.84±0.04 µg/g; in maize it was recorded as 4.28 ± 0.01 µg/g to 2.98 ± 0.04 µg/g and also in wheat to about 4.24 ± 0.02 µg/g to 2.54 ± 0.02 µg/g respectively.

Nickel has been considered to be an trace essential trace element for human (Animal) health (Zhuang et al., 2012). The permissible tolerable limit in agricultural crops is 50µg/g and normal is about 0.1 to 5.0µg/g. The mean concentration of Ni level in sugarcane collected from 5 to 50 mt from the edge of road was recorded as 4.29 ± 0.02 µg/g to 0.76 ± 0.01µg/g, in maize it was 2.92 ± 0.02 µg/g to 0.82 ± 0.01 µg/g and also in wheat it was 2.82 ± 0.01 µg/g to 0.76 ± 0.01 µg/g respectively. Nickel occurs mainly in the form of Sulphide and silicate minerals. Ni when administrated to animals is rapidly distributed to kidneys, pituitary, lungs, skin, adrinals, ovaries and testis (Sundarman-1989). Ni is carcinogenic to human and risks are highest for lung and nasal cancers. Ni also damages DNA directly through reactive oxygen species (McCoy and Kinney,1992).

CONCLUSION

Based in the analysis and results, it could be concluded that study on roadside soil, test plants and crops confirmed that vehicular emission is potential source of environmental pollution. The high level concentration Lead, Cadmium and Nickel concentration in soil will affect the health of the residents as well as surrounding communities, which may also affect soil fertility too. The consumption of these crops can considered safe with no risk to human health. The average intake of metals in long time low level body accumulation of heavy metals and detrimental impact becomes apparent only several year of exposure. These findings also suggest that special attention should be taken to this traffic related environmental issue and further suggest that serious affords required to reduced the high level of soil remediation and before the consumption of crops/vegetables should washed to remove significant amount of aerial accumulation from the surface of crops/vegetables. Finally, it is recommended that economical plant (vegetable/crops) should not be cultivated along the roadside and especially in high traffic density areas.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Com.BHS Arts and TGP Science College, Jamkhandi (Karnataka), Principal, B.V.V. Snaghas, Basaveshwar Science College Bagalkot (Karnataka), Chairman, PG Department Botany, Karnataka University, Dharawad (Karnataka) for providing necessary facilities to carry out research work.

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ISSN: 0976-3031

Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 08 (B), pp. 39483-39488, August, 2020

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOTOOL TO MONITOR HEAVY METAL POLLUTION IN ROADSIDE SOIL, GRASS, FICUS AND SOME ECONOMICALLY IMPORTANT CROPS

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1108.5512

ARTICLE INFO

Article History:

Received 24th May, 2020
Received in revised form 19th June, 2020
Accepted 25th July, 2020
Published online 28th August, 2020

Key Words:

Xenobiotics , Ficus, Crops, Grass, Accumulation, Bioindicators, Health

ABSTRACT

Heavy metals are important environmental pollutants and their toxicity in human, plants and animals has been received much more attention. A study was conducted to investigate the heavy metal pollution roadside soil, grass, ficus species and also some economically important crops along National highway No.4 with heavy traffic load passing along the sides from Jamkhandi to Mudhol (India). The highest levels of metal concentration of lead, cadmium, manganese, zinc, chromium and Nickel were found in the samples from very traffic congestion and were determined by using Atomic Absorption Spectrophotometer (AAS). The soil samples at a depth (0-20 cm) grass, ficus and some economically important crop leaves (wheat, maize, sugarcane) were taken from different sapling sites viz, S_1, S_2, S_3, S_4 and S_5 on state highway with high traffic road passing from Jamkhandi to Mudhol and were determined by AAS. The results showed that soil, grass, ficus and crops also contains elevated levels of metal. It was found that the primary source of the contamination occurs mainly by the vehicular exhausts. The increased circulation of toxic metals in soil, grass, ficus and crop results in the inevitable build up of xenibiotics in the food chain. The variation in heavy metal concentration is due to the changes in traffic density and anthropogenic activities . From the results it is concluded that the grass, ficus, crop plants and soil samples were used as bioindicators of metal pollution.

INTRODUCTION

Toxic level of heavy metals can cause damage to the ecology environmental nutritional and evolutionary characteristic of polluted area and consequently human residing along these areas is constantly exposed health risk (Yuan et al., 2015; Kumar et al., 2017; Zheng, 2017). Soil-plant systems to make able human productivity but suffer from pollution damage caused by human activities (Assirey and El-Shahawi, 2015; Rolli et al., 2015; Wang et al.,2017) and with the rapid development of National ecology and the subsequently traffic pollution, negative environment effect are becoming increasing apparent especially roadside plant system soil (Seedi et al., 2009; Galal and Shehata, 2015; Yang et al., 2015). Vehicular emission considered as main source of heavy metals such as Pb, Cd, Ni, Fe and Cu (Radziemska and Fronczyk, 2015; Al-fawwaz and Al-Khazaleh, 2017). The high concentration of heavy metals in urban roadside and plant samples influenced by ecological conditions like wind, rainfall, land and traffic densities (Sheikh, et al., 2016). The level of heavy metal in soil and plant inversely related with increase of distance from road edge (Kumar and Kumar, 2017). Accumulation of heavy metals in roadside soil can alter biological activities in soil and affect the enzymatic activity of microorganisms such as urease and phosphate (Flughes et al., 1980; Kumar and Kumar, 2017). Heavy metals have complex relation with plant. Histidine, citric acid, malic acid and oxalic acid present in the plant form complexes with heavy metals and convert the metals into nontoxic form (McGrah, 1994; Agarwal et al., 2007). Consumption of such contaminated crops may pose a health risk to human beings as metals form complexes with -COOH, -NH2, -SH, > NH groups present in protein to catalyse the function of enzyme (Kumar and Kumar, 2017). The new biological complexes thus formed lose their function which result in breakdown and even damage to cell also (Pirsaheb et al., 2013; Kumar and Kumar, 2017). Due to non-biodegradable and persistent nature of heavy metal, they easily accumulated in soft tissue of human being and can cause disturbance of biological process and can cause cardiovascular, kidney, liver and bone diseases (Momodu and Anyakosa, 2010; Kumar and Kumar, 2015). Information on accumulation of heavy metal on roadside soil of this study area is due to highway traffic and vehicles (Pirsaheb et al., 2013). This could be a new threat for

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agriculture. Determination of heavy metal accumulation in roadside soil , plant leaves and crop leaves may be the index of the environmental pollution of Mudhol and Jamkhandi area . Keeping this view in mind, the research was conducted to know the heavy metal accumulation of roadside soil, grass, ficus and economically important crops of the roadside and also their effect on health of the organisms.

MATERIALS AND METHODS

Jamkhandi is the city of Northern region of Karnataka at longitude 1630′ 6″ N and latitude -7516′ 17″. The city high between Jamkhandi to Mudhol is suffering from high traffic density caused by the vehicles. The grass, ficus, crop plant viz, maize, sugarcane, wheat and soil were collected, which were three meters away from the state highway (Fig. Table. 1). Grass, ficus and samples were collected from each state at three random spots that were spaced approximately at one interval. Similarly three crop plant leaves are taken at 5m, 25m, 50m and 1000m away from the grass, ficus site in triplicate. The leaves were clipped with stainless steel scissors.

The leaves of grass (*Cyanodon dactylon* L.), Ficus (*Ficus bengalensis* L.) and crops viz., Wheat (*Triticum sativum* L.), Maize (*Zea mays* L.) and Sugarcane (*Saccharum officinarum* L.) samples were dried at 80^0C for 48 hrs and was powdered and sieved through 0.2 mm sieve one gram of each sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method (mixed acid digestion method). The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made up to 100 ml. Similarly soil samples were dried, powdered and sieved through 0.2 mm sieve one gram of sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method. The resulting extract were diluted and filtered through Whattman No 41 paper and was made up to 100 ml using double distilled water and analyzed for heavy metals viz, Lead (Pb, 217.0nm), Cadmium (Cd, 228.8 nm), Copper (Cu, 324.7nm), Zinc (Zn, 213.9nm), Manganese (Mn, 279.5nm), Nickel (Ni, 232.0nm), and Chromium (Cr, 221.8 nm) filters (respective wavelengths) have been used for the estimation using Atomic Absorption Spectrophotometer (GBC 932 plus AAS, Austrelia). The working standards were prepared by serial dilution of standard stock solutions and were used for the calibration of the instrument (Pirsaheb et al., 2013).

Table 1 Description of sampling stations along the state highway of Jamkhandi to Mudhol

Sampling station		Nature of station
Control	Jamkhandi	Unpolluted area- Vehicular movement is negligible unpolluted area with less disturbance.
1	Jamkhandi bypass road	Vehicular movement is high.
2	Siddapur	Vehicular movement is high – Agricultural fields on either side of the road.
3	Prabhulingeshwar Sugar factory station	Vehicular movement is high - Agricultural fields on either side of the road but sugar factory is far away from the state highway.
4	Shirol cross	Vehicular movement is high – Agricultural fields on either side.
5	Malapur	Vehicular movement is high – Agricultural fields on either side.
6	Mudhol	Vehicular movement is high – Agricultural fields on either side & Nirani sugar factory is far away from the state highway

Table 2 Correlation coefficient of heavy metals in roadside soil and grass

S.NO	Metal	r-value
1	Lead	0.639*
2	Copper	0.478
3	Zinc	0.828*
4	Cadmium	0.748*
5	Manganese	0.531
6	Nickel	0.335
7	Chromium	0.208

Significant at **5%** level (P>0.05)
r=0.60 & above have significant correlation

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus

S.NO	**Metal**	**r-value**
1	Lead	0.641*
2	Copper	0.480
3	Zinc	0.826*
4	Cadmium	0.742*
5	Manganese	0.524
6	Nickel	0.327
7	Chromium	0.202

Significant at **5%**level(P0.05)
r=0.60 & above have significant correlation

RESULTS AND DISCUSSIONS

Pollution by heavy metals such as Pb, Cd, Ni, Cr etc is a pollution of concern (Onder and Dursun, 2006). So it has become necessary to conduct this experiment (study) to exhibit and determine the kind of environmental pollution and how far they exhibit and efficient as a bioindicator in reducing the degree of pollution in environment. The level of heavy metals in the plant and crop samples collected along the roadside (fig. 1). Correlation coefficient of heavy metals in roadside soil, grass and ficus plant samples are given in Table 2 and 3. Mean concentration of heavy metals (µg/g) and ± standard deviation in the crops is given the table 4.The ranges and arthematic mean of heavy metal concentration of soil, grass and ficus samples of state highway and control sites are presented in the table -4.

Lead is one of the major heavy metal and is considered as an environmental pollutant (Sharma and Dubey, 2005). Pb is considered as a general protoplasmic poison which accumulate and slowly acting.

The main source of Pb is exhaust fumes of automobiles, chimneys of factory, road side vehicles pollution (Eick et al., 1999). The results of our analysis show that there are significant differences for lead between sampling sites in control and polluted area. The results shows that soil tends to accumulate more Pb than grass and ficus leaves and the highest Pb level found in the roadside soil was 142.40µg/g, while the ficus, it was found that 27.38 µg/g similarly in grass it was 28.32µg/g. The mean soil Pb level of 96.74µg/g indicated considerable contamination of metal in the roadside environment, whereas, control soil has a baseline level of 72.24µg/g Pb. Much of the lead is rapidly washed on to the soil by rain water from the surface and also by the death and decomposition of the plant. The Pb deposited on soils and vegetation can also cause enhanced levels of Pb in soil microorganisms (Harrison et al., 1981; Khattak et al., 2013).

Table 4 Heavy metal accumulation profile in roadside grass, ficus and soil

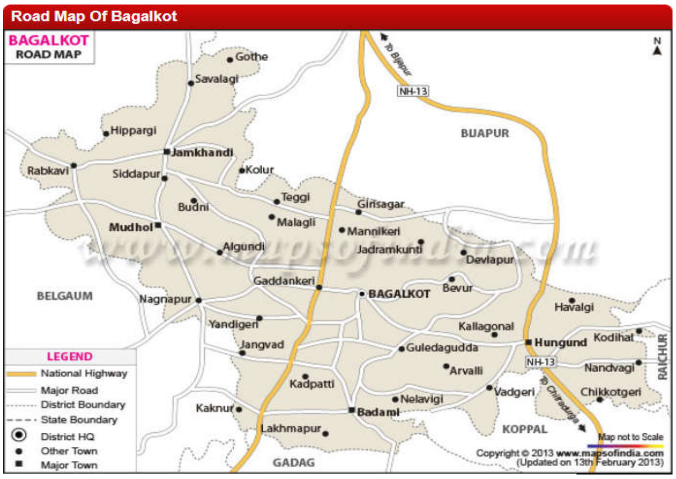
SI. NO	Heavy metals	Control group µg/g (dry wt)	Roadside grass µg/g (dry wt)		Control group µg/g (dry wt)	Roadside Ficus µg/g (dry wt)		Control group µg/g (dry wt)	Roadside soil µg/g (dry wt)	
			Range	**Mean± SE**	20.42	Range	**Mean± SE**		Range	Mean±SE
1	Lead	20.42	20.42 - 28.32	23.722 ±1.81	2.14	20.22 - 27.38	23.72 ±1.82	72.24	84.60-142.4	96.74**±8.66**
2	Copper	2.12	3.93 - 5.72	4.878 ± 0.32	15.178	3.92 - 5.72	4.70 ± 0.34	36.8	39.88-61.26	49.98**±3.3**
3	Zinc	15.173	24.48 - 34.16	32.878 ±3.11	0.88	24.42 - 36.7	30.84 ±3.10	32.0	34.26-398.02	188.8**±54.28**
4	Cadmium	0.88	1.20 - 1.78	1.594 ±0.085	16.22	1.12 - 1.78	1.42 ±0.06	2.08	1.72-2.84	2.4**±0.18**
5	Manganese	16.18	28.88 - 74.18	56.804 ±7.35	N.D	28.02 - 72.10	56.10 ±7.31	1261.42	1262.80-2034.8	1542.34**±26.59**
6	cadmium	N.D*	1.30-9.00	4.89±2.23	7.22	1.20 - 8.6	4.62 ± 2.20	124.42	129.4-962.0	326.5**±2.46**
7	Nickel	7.16	8.6 – 16.02	10.948 ±1.42		8.6 – 16.08	9.12 ± 1.42	71	74.53-118.60	88.98**±6.35**

ND* - Not detectable

Table 5 Mean concentration of heavy metals (µg/g) and ± standard deviation in crops at Shirol

Metals	**Sugarcane (Distance in mt)**				**Maize (Distance in mt)**				**Wheat (Distance in mt)**			
	5	**25**	**50**	**100**	**5**	**25**	**50**	**100**	**5**	**25**	**50**	**100**
Pb	22.72±1.81	16.42±0.02	8.12±0.02	0.08±0.02	18.21±0.03	10.21±0.02	4.26±0.02	0.08±0.01	15.72±0.02	8.21±0.02	333.27±0.07	**0.7**±0.01
Cu	4.93±0.02	4.24±0.02	3.04±0.02	2.15±0.01	4.94±0.02	4.32±0.02	3.82±0.01	2.92±0.01	4.82±0.07	4.28±0.02	3.92±0.01	2.94±0.0
Zn	32.84±0.01	20.21±0.02	22.04±0.02	14.02±0.01	30.98±0.02	24.2±0.02	16.02±0.04	12.02±0.01	31.004±0.02	22.04±0.02	18.42±0.04	12.08±0.01
Cd	1.54±0.02	1.22±0.02	1.02±0.04	0.88±0.01	1.64±0.01	1.24±0.02	0.86±0.01	0.68±0.02	1.32±0.03	1.24±0.02	0.88±0.01	0.64±0.06
Mn	56.12±0.01	38.72±0.02	28.12±0.04	15.28±0.04	52.08±0.02	46.82±0.01	36.28±0.02	18.28±0.01	53.28±0.02	41.28±0.01	32.18±0.01	16.22±0.02
Cr	4.61±0.01	4.02±0.03	3.84±0.04	1.82±0.03	4.28±0.01	3.84±0.04	2.98±0.04	1.20±0.05	4.24±0.02	3.84±0.04	2.54±0.02	1.24±0.05
Ni	4.29±0.02	2.62±0.02	0.76±0.01	0.07±0.01	2.92±0.02	1.62±0.02	0.82±0.01	0.071±0.01	2.82±0.01	1.58±0.03	0.76±0.01	0.68±0.03

Fig 1 Map showing the National Highway No. 4 passing between Jamkhandi to Mudhol



Roadside soil gave higher concentration of Cu due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of cars derived from engine wear, brussing and bearing metals (Al-Khashman, 2007). The mean Cu level in roadside soil 49.98µg/g was found to be much higher the grass 4.87µg/g and ficus 4.70µg/g.

The source of zinc in relation to automobile traffic is wearing of break lining, looses of oil and cooling liquid (Saeedi et al., 2009). Arithematic mean of Zn of the roadside soil of around Jamkhandi shows a relatively high level of 188.8µg/g with a range of 34.20µg/g -398.02µg/g. The range of Zn 24.42 µg/g – 36.7µg/g found in ficus and grass 24.48 µg/g – 34.16µg/g (roadside) is not much higher. This can be attributed to the fact that Zn as an essential element is normally in uncontaminated plants up to 100 µg/g (Ho and Tai, 1988).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process , thus, plants can easily absorbs Cd from soil and transport to the shoot system.

Cadmium induces complex changes in plants genetically, biochemical and physiological levels. Our analysis for Cd in the roadside plants and control area. Cadmium level in the roadside soil averaged about 2.4µg/g and was the lowest among the seven metals examined. The mean Cd in ficus 1.42µg/g and in grass 1.594µg/g. Our finding are in confirmation with findings of (Ho and Tai, 1988).

The soil, grass and ficus contained much higher levels of Mn than other metals examined. Roadside soil, grass and ficus had average 1542µg/g, 56.804µg/m and 56.10µg/g of Mn content of the roadside soil may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil. Chromium is considered as a serious pollutant due to wide industrial use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are determined to their growth and development. Significant differences in our analysis for Cr in soil and in plant samples are found. Chromium level too was very high in roadside soil (326.5µg/g) against the control value of 124.42µg/g. In grass it was 4.89µg/g and in ficus it was found to be 4.62µg/g against control (Zero). Nickel level was considerable and was in roadside soil (88.98 µg/g) against control value (71.0 µg/g). In grass it was 10.94µg/g and in ficus, it was found that 9.12µg/g against control (7.16µg/g).

Simple linear regression between the metals viz, Pb, Cu, Ni, Mn, Zn, Cd and Cr present in the soil, grass and ficus were calculated and are given in the Tables 3and 4.

According to simple linear regression between the metal levels in roadside soil and ficus were found in Zn, Cd and Ni are significant at 5% level ($P < 0.05$). It may be indicating the bio-

concentration of these metals in the ficus, in addition to aerial deposition. This may be attributed to the favourable root environment (Sahu and Warrier, 1985) i.e, soil conditions might have favored their absorption.

Simple linear regression in case of chromium, nickel, manganese and copper contents between the soil, grass and ficus are not significant at 5% level, were low due to low bioavailability of these metals owing to unfavorable root environment. Whatever excess content of these metals found in soil, grass and ficus was pressured to be due to aerial deposition contributed by motor vehicles and other anthropogenic activities.

The order of increment of heavy metals in roadside is as follows

Soil: Mn > Cr > Zn > Pb > Ni > Cu > Cd
Grass: Mn > Zn > Pb > Ni > Cr > Cu > Cd and
Ficus: Mn > Zn > Pb > Ni > Cu > Cr > Cd.

The elevated levels of heavy metals in the road side soil and ficus is an indication of airborne pollutants of road side environment of the urban area of Jamkhandi city and along the road soil has high retention capacity for the heavy metals (Yassoglou, et al., 1987) due to there cation exchange capacity (CFC), complexing organic substances, oxides and carbonates. Thus, contamination levels increase continuously as long as the nearby sources remain active. During the last two decades, the city of Jamkhandi to the extent has witnessed sharp increase in vehicle number due to urbanization. Similar observation in Neem and Caesalpinia in mudhurai city of southern region of Tamil Nadu (Thambavani and Vanthana, 2013) .

In soil, the lesser mobility of metals and its accumulation on a long term basis, leads to overall higher contamination level of metals, Whereas, in roadside grass, ficus represents more accumulation due to turnover of plant materials (like new growths, the senescence followed by the abscission of old parts) and meterological influence (Kabata-Pendias, 2005). Thus , the study of metal concentration of roadside soil, grass and ficus reflects the extent of aerial contamination of roadside environment. The penetration of heavy metals into the food chains due to vehicular emissions may cause a long-range ecological and health hazard.

Accumulation profile of heavy metals in Crops

There are significant differences between the distribution of heavy metals in the crops at different Sampling station with varying distances (Table. 5). The accumulation of heavy metals was found to be high in all test crops at different locations compare to control and found in the order of 5 mt > 25mt > 50mt > 1000mt (control). The mean concentration of Pb level in test sugarcane collected from 5 to 50mt from the edge of road was recorded as 22.72 ± 1.81µg/g to 8.12 ± 0.03µg/g in maize it was recorded as 18.21 ± 0.03 µg/g to 4.26 ±0.02µg/g and in wheat it was recorded as 15.72 ± 0.02 µg/g to 3.27 ± 0.07µg/g, which was significantly higher than Indian standard (2.5µg/g) recommended by Awasthi, (2000). The permissible tolerable limit in agricultural crops is 10.0 µg/g and normal is varying from 5.0 to 15.0µg/g (Kabuta-Pendias 2005).

Lead is a poisonous metal, in human it is directly absorbed in to blood stream and is stored soft tissues, bones and teeth. Due to bioaccumulation it leads to chronic damage to central nervous system (CNS) and peripheral nervous system (PNS) and also brings difficulties in pregnancy (Peokjoo et al., 2008). It includes aberrant gene transcription (Boutan et al., 2001)

The mean concentration of Cu level in test sugar cane collected from 5 to 50mt from the edge of the road was recorded as 4.93 ± 0.02 µg/g to 3.04 ± 0.02 µg/g, in maize it was recorded as 4.94 ± 0.02 µg/g to 3.82 ± 0.01 µg/g and also in wheat it was recorded 4.82 ± 0.07 µg/g to 3.92 ± 0.01 µg/g which was significantly lower than tolerable limit in agricultural crops for Cu is 50µg/g and normal limit is about 5-30µg/g (Kabuta-Pendias 2005) copper is essential element but higher concentration intake leads to severe mucosal irritation, widespread capillary damage (Salmeron and Pozo, 1989).

The tolerable limit of agricultural crops for Zinc is 300 µg/g and normal is 27-150µg/g. The mean concentration of Zinc level in sugarcane collected from 5 to 50 mt from the edge of the road was recorded as 32.81 ± 0.01µg/g to 22.04 ± 0.03 µg/g, in maize recorded as 30.98 ± 0.02µg/g to 16.02 ± 0.04µg/g and also in wheat it was 31.04 ± 0.02 µg/g to 18.42 ± 0.04 µg/g respectively.

Zinc is considered to be relatively nontoxic, however, excess amount can cause system dysfunctions that results in impairment of growth and reproduction (Dubey et al., 2007). Excess concentration of metal in the body bound in various transcription regions such as polymerase enzymes (Wang et al., 1997).

Manganese is micronutrient , essential for physiological functions. The tolerable limit for Mn in agricultural crops is 300µg/g and normal value is 30 to 300 µg/g (Kabuta-Pendias 2005). The mean concentration of Mn level in sugarcane collected from 5 to 50 mt from the edge of rod was recorded as 50.12 ± 0.01 µg/g to 28.12 ± 0.04 µg/g, in maize it was recorded as 52.08 ± 0.02 µg/g to 36.28 ± 0.02 µg/g and also in wheat it was recorded as 53.28 ± 0.02 µg/g to 32.18 ± 0.01 µg/g respectively. Mn concentrations in test crops lower than upper limit recommended by Kabuta-Pendias (2005). But higher concentration is toxic causing neuropscychiatic disorder characterized by irritability, difficulty in Walking and Speech disturbances (Singh and Kalmadhad, 2011).

The permissible tolerable limit in agricultural crops for Cd is 3.0 µg/g and normal is varying from 0.05 to 0.2 µg/g (Kabuta-Pendias 2005).In control (1000mt) crop plants maximum accumulation is recorded in sugar (0.88 ± 0.01µg/g) and minimum is 0.64 ± 0.06µg/g in wheat.

Cadmium accumulate in the human kidney, respiratory system, cardiac failure and is also associated with bone diseases (Singh and Kalamdhad-2011). (Wang and Crowley 2005) also reported that discruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of Cd-toxicity Cd level in sugar collected from 5 to 50 mt from the edge of the road was recorded as 1.54 ± 0.02 µg/g to 1.02 ± 0.04 µg/g, in maize it was recorded as 1.64 ± 0.01 µg/g to 0.86 ± 0.01µg/g and also it was recorded to about 1.32 ± 0.03 µg/g to 0.88 ± 0.04µg/g in wheat respectively.

Chromium is considered as a serious environmental pollutant, due to industrial (wide) use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are detrimental to their growth. The mean concentration of Cr level in sugarcane

collected from 5 to 50 mt from the edge of road was recorded as 4.61±0.01 µg/g to 3.84±0.04 µg/g; in maize it was recorded as 4.28 ± 0.01 µg/g to 2.98 ± 0.04 µg/g and also in wheat to about 4.24 ± 0.02 µg/g to 2.54 ± 0.02 µg/g respectively.

Nickel has been considered to be an trace essential trace element for human (Animal) health (Zhuang et al., 2012). The permissible tolerable limit in agricultural crops is 50µg/g and normal is about 0.1 to 5.0µg/g. The mean concentration of Ni level in sugarcane collected from 5 to 50 mt from the edge of road was recorded as 4.29 ± 0.02 µg/g to 0.76 ± 0.01µg/g, in maize it was 2.92 ± 0.02 µg/g to 0.82 ± 0.01 µg/g and also in wheat it was 2.82 ± 0.01 µg/g to 0.76 ± 0.01 µg/g respectively. Nickel occurs mainly in the form of Sulphide and silicate minerals. Ni when administrated to animals is rapidly distributed to kidneys, pituitary, lungs, skin, adrinals, ovaries and testis (Sundarman-1989). Ni is carcinogenic to human and risks are highest for lung and nasal cancers. Ni also damages DNA directly through reactive oxygen species (McCoy and Kinney,1992).

CONCLUSION

Based in the analysis and results, it could be concluded that study on roadside soil, test plants and crops confirmed that vehicular emission is potential source of environmental pollution. The high level concentration Lead, Cadmium and Nickel concentration in soil will affect the health of the residents as well as surrounding communities, which may also affect soil fertility too. The consumption of these crops can considered safe with no risk to human health. The average intake of metals in long time low level body accumulation of heavy metals and detrimental impact becomes apparent only several year of exposure. These findings also suggest that special attention should be taken to this traffic related environmental issue and further suggest that serious affords required to reduced the high level of soil remediation and before the consumption of crops/vegetables should washed to remove significant amount of aerial accumulation from the surface of crops/vegetables. Finally, it is recommended that economical plant (vegetable/crops) should not be cultivated along the roadside and especially in high traffic density areas.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Com.BHS Arts and TGP Science College, Jamkhandi (Karnataka), Principal, B.V.V. Snaghas, Basaveshwar Science College Bagalkot (Karnataka), Chairman, PG Department Botany, Karnataka University, Dharawad (Karnataka) for providing necessary facilities to carry out research work.

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 11, Issue, 08 (B), pp. 39483-39488, August, 2020

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOTOOL TO MONITOR HEAVY METAL POLLUTION IN ROADSIDE SOIL, GRASS, FICUS AND SOME ECONOMICALLY IMPORTANT CROPS

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DOI: http://dx.doi.org/10.24327/ijrsr.2020.1108.5512

ARTICLE INFO

Article History:

Received 24th May, 2020
Received in revised form 19th June, 2020
Accepted 25th July, 2020
Published online 28th August, 2020

Key Words:

Xenobiotics , Ficus, Crops, Grass, Accumulation, Bioindicators, Health

ABSTRACT

Heavy metals are important environmental pollutants and their toxicity in human, plants and animals has been received much more attention. A study was conducted to investigate the heavy metal pollution roadside soil, grass, ficus species and also some economically important crops along National highway No.4 with heavy traffic load passing along the sides from Jamkhandi to Mudhol (India). The highest levels of metal concentration of lead, cadmium, manganese, zinc, chromium and Nickel were found in the samples from very traffic congestion and were determined by using Atomic Absorption Spectrophotometer (AAS). The soil samples at a depth (0-20 cm) grass, ficus and some economically important crop leaves (wheat, maize, sugarcane) were taken from different sapling sites viz, S_1, S_2, S_3, S_4 and S_5 on state highway with high traffic road passing from Jamkhandi to Mudhol and were determined by AAS. The results showed that soil, grass, ficus and crops also contains elevated levels of metal. It was found that the primary source of the contamination occurs mainly by the vehicular exhausts. The increased circulation of toxic metals in soil, grass, ficus and crop results in the inevitable build up of xenibiotics in the food chain. The variation in heavy metal concentration is due to the changes in traffic density and anthropogenic activities . From the results it is concluded that the grass, ficus, crop plants and soil samples were used as bioindicators of metal pollution.

INTRODUCTION

Toxic level of heavy metals can cause damage to the ecology environmental nutritional and evolutionary characteristic of polluted area and consequently human residing along these areas is constantly exposed health risk (Yuan et al., 2015; Kumar et al., 2017; Zheng, 2017). Soil-plant systems to make able human productivity but suffer from pollution damage caused by human activities (Assirey and El-Shahawi, 2015; Rolli et al., 2015; Wang et al.,2017) and with the rapid development of National ecology and the subsequently traffic pollution, negative environment effect are becoming increasing apparent especially roadside plant system soil (Seedi et al., 2009; Galal and Shehata, 2015; Yang et al., 2015). Vehicular emission considered as main source of heavy metals such as Pb, Cd, Ni, Fe and Cu (Radziemska and Fronczyk, 2015; Al-fawwaz and Al-Khazaleh, 2017). The high concentration of heavy metals in urban roadside and plant samples influenced by ecological conditions like wind, rainfall, land and traffic densities (Sheikh, et al., 2016). The level of heavy metal in soil and plant inversely related with increase of distance from road edge (Kumar and Kumar, 2017). Accumulation of heavy metals in roadside soil can alter biological activities in soil and affect the enzymatic activity of microorganisms such as urease and phosphate (Flughes et al., 1980; Kumar and Kumar, 2017). Heavy metals have complex relation with plant. Histidine, citric acid, malic acid and oxalic acid present in the plant form complexes with heavy metals and convert the metals into nontoxic form (McGrah, 1994; Agarwal et al., 2007). Consumption of such contaminated crops may pose a health risk to human beings as metals form complexes with -COOH, -NH2, -SH, > NH groups present in protein to catalyse the function of enzyme (Kumar and Kumar, 2017). The new biological complexes thus formed lose their function which result in breakdown and even damage to cell also (Pirsaheb et al., 2013; Kumar and Kumar, 2017). Due to non-biodegradable and persistent nature of heavy metal, they easily accumulated in soft tissue of human being and can cause disturbance of biological process and can cause cardiovascular, kidney, liver and bone diseases (Momodu and Anyakosa, 2010; Kumar and Kumar, 2015). Information on accumulation of heavy metal on roadside soil of this study area is due to highway traffic and vehicles (Pirsaheb et al., 2013). This could be a new threat for

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agriculture. Determination of heavy metal accumulation in roadside soil , plant leaves and crop leaves may be the index of the environmental pollution of Mudhol and Jamkhandi area . Keeping this view in mind, the research was conducted to know the heavy metal accumulation of roadside soil, grass, ficus and economically important crops of the roadside and also their effect on health of the organisms.

MATERIALS AND METHODS

Jamkhandi is the city of Northern region of Karnataka at longitude 1630′ 6″ N and latitude -7516′ 17″. The city high between Jamkhandi to Mudhol is suffering from high traffic density caused by the vehicles. The grass, ficus, crop plant viz, maize, sugarcane, wheat and soil were collected, which were three meters away from the state highway (Fig. Table. 1). Grass, ficus and samples were collected from each state at three random spots that were spaced approximately at one interval. Similarly three crop plant leaves are taken at 5m, 25m, 50m and 1000m away from the grass, ficus site in triplicate. The leaves were clipped with stainless steel scissors.

The leaves of grass (*Cyanodon dactylon* L.), Ficus (*Ficus bengalensis* L.) and crops viz., Wheat (*Triticum sativum* L.), Maize (*Zea mays* L.) and Sugarcane (*Saccharum officinarum* L.) samples were dried at 80^0C for 48 hrs and was powdered and sieved through 0.2 mm sieve one gram of each sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method (mixed acid digestion method). The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made up to 100 ml. Similarly soil samples were dried, powdered and sieved through 0.2 mm sieve one gram of sample was digested using Gerhardt digestion unit according to Allen et al., (1974) method. The resulting extract were diluted and filtered through Whattman No 41 paper and was made up to 100 ml using double distilled water and analyzed for heavy metals viz, Lead (Pb, 217.0nm), Cadmium (Cd, 228.8 nm), Copper (Cu, 324.7nm), Zinc (Zn, 213.9nm), Manganese (Mn, 279.5nm), Nickel (Ni, 232.0nm), and Chromium (Cr, 221.8 nm) filters (respective wavelengths) have been used for the estimation using Atomic Absorption Spectrophotometer (GBC 932 plus AAS, Austrelia). The working standards were prepared by serial dilution of standard stock solutions and were used for the calibration of the instrument (Pirsaheb et al., 2013).

Table 1 Description of sampling stations along the state highway of Jamkhandi to Mudhol

Sampling station		Nature of station
Control	Jamkhandi	Unpolluted area- Vehicular movement is negligible unpolluted area with less disturbance.
1	Jamkhandi bypass road	Vehicular movement is high.
2	Siddapur	Vehicular movement is high – Agricultural fields on either side of the road.
3	Prabhulingeshwar Sugar factory station	Vehicular movement is high - Agricultural fields on either side of the road but sugar factory is far away from the state highway.
4	Shirol cross	Vehicular movement is high – Agricultural fields on either side.
5	Malapur	Vehicular movement is high – Agricultural fields on either side.
6	Mudhol	Vehicular movement is high – Agricultural fields on either side & Nirani sugar factory is far away from the state highway

Table 2 Correlation coefficient of heavy metals in roadside soil and grass

S.NO	Metal	r-value
1	Lead	0.639*
2	Copper	0.478
3	Zinc	0.828*
4	Cadmium	0.748*
5	Manganese	0.531
6	Nickel	0.335
7	Chromium	0.208

Significant at **5%** level (P>0.05)
r=0.60 & above have significant correlation

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus

S.NO	**Metal**	**r-value**
1	Lead	0.641*
2	Copper	0.480
3	Zinc	0.826*
4	Cadmium	0.742*
5	Manganese	0.524
6	Nickel	0.327
7	Chromium	0.202

Significant at **5%**level(P0.05)
r=0.60 & above have significant correlation

RESULTS AND DISCUSSIONS

Pollution by heavy metals such as Pb, Cd, Ni, Cr etc is a pollution of concern (Onder and Dursun, 2006). So it has become necessary to conduct this experiment (study) to exhibit and determine the kind of environmental pollution and how far they exhibit and efficient as a bioindicator in reducing the degree of pollution in environment. The level of heavy metals in the plant and crop samples collected along the roadside (fig. 1). Correlation coefficient of heavy metals in roadside soil, grass and ficus plant samples are given in Table 2 and 3. Mean concentration of heavy metals (µg/g) and ± standard deviation in the crops is given the table 4.The ranges and arthematic mean of heavy metal concentration of soil, grass and ficus samples of state highway and control sites are presented in the table -4.

Lead is one of the major heavy metal and is considered as an environmental pollutant (Sharma and Dubey, 2005). Pb is considered as a general protoplasmic poison which accumulate and slowly acting.

The main source of Pb is exhaust fumes of automobiles, chimneys of factory, road side vehicles pollution (Eick et al., 1999). The results of our analysis show that there are significant differences for lead between sampling sites in control and polluted area. The results shows that soil tends to accumulate more Pb than grass and ficus leaves and the highest Pb level found in the roadside soil was 142.40µg/g, while the ficus, it was found that 27.38 µg/g similarly in grass it was 28.32µg/g. The mean soil Pb level of 96.74µg/g indicated considerable contamination of metal in the roadside environment, whereas, control soil has a baseline level of 72.24µg/g Pb. Much of the lead is rapidly washed on to the soil by rain water from the surface and also by the death and decomposition of the plant. The Pb deposited on soils and vegetation can also cause enhanced levels of Pb in soil microorganisms (Harrison et al., 1981; Khattak et al., 2013).

Table 4 Heavy metal accumulation profile in roadside grass, ficus and soil

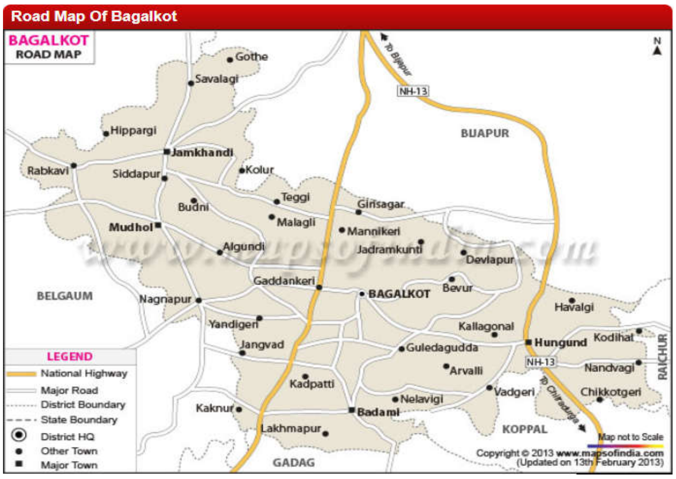
SI. NO	Heavy metals	Control group µg/g (dry wt)	Roadside grass µg/g (dry wt)		Control group µg/g (dry wt)	Roadside Ficus µg/g (dry wt)		Control group µg/g (dry wt)	Roadside soil µg/g (dry wt)	
			Range	**Mean± SE**	20.42	Range	**Mean± SE**		Range	Mean±SE
1	Lead	20.42	20.42 - 28.32	23.722 ±1.81	2.14	20.22 - 27.38	23.72 ±1.82	72.24	84.60-142.4	96.74**±8.66**
2	Copper	2.12	3.93 - 5.72	4.878 ± 0.32	15.178	3.92 - 5.72	4.70 ± 0.34	36.8	39.88-61.26	49.98**±3.3**
3	Zinc	15.173	24.48 - 34.16	32.878 ±3.11	0.88	24.42 - 36.7	30.84 ±3.10	32.0	34.26-398.02	188.8**±54.28**
4	Cadmium	0.88	1.20 - 1.78	1.594 ±0.085	16.22	1.12 - 1.78	1.42 ±0.06	2.08	1.72-2.84	2.4**±0.18**
5	Manganese	16.18	28.88 - 74.18	56.804 ±7.35	N.D	28.02 - 72.10	56.10 ±7.31	1261.42	1262.80-2034.8	1542.34**±26.59**
6	cadmium	N.D*	1.30-9.00	4.89±2.23	7.22	1.20 - 8.6	4.62 ± 2.20	124.42	129.4-962.0	326.5**±2.46**
7	Nickel	7.16	8.6 – 16.02	10.948 ±1.42		8.6 – 16.08	9.12 ± 1.42	71	74.53-118.60	88.98**±6.35**

ND* - Not detectable

Table 5 Mean concentration of heavy metals (µg/g) and ± standard deviation in crops at Shirol

Metals	**Sugarcane (Distance in mt)**				**Maize (Distance in mt)**				**Wheat (Distance in mt)**			
	5	**25**	**50**	**100**	**5**	**25**	**50**	**100**	**5**	**25**	**50**	**100**
Pb	22.72±1.81	16.42±0.02	8.12±0.02	0.08±0.02	18.21±0.03	10.21±0.02	4.26±0.02	0.08±0.01	15.72±0.02	8.21±0.02	333.27±0.07	**0.7**±0.01
Cu	4.93±0.02	4.24±0.02	3.04±0.02	2.15±0.01	4.94±0.02	4.32±0.02	3.82±0.01	2.92±0.01	4.82±0.07	4.28±0.02	3.92±0.01	2.94±0.0
Zn	32.84±0.01	20.21±0.02	22.04±0.02	14.02±0.01	30.98±0.02	24.2±0.02	16.02±0.04	12.02±0.01	31.004±0.02	22.04±0.02	18.42±0.04	12.08±0.01
Cd	1.54±0.02	1.22±0.02	1.02±0.04	0.88±0.01	1.64±0.01	1.24±0.02	0.86±0.01	0.68±0.02	1.32±0.03	1.24±0.02	0.88±0.01	0.64±0.06
Mn	56.12±0.01	38.72±0.02	28.12±0.04	15.28±0.04	52.08±0.02	46.82±0.01	36.28±0.02	18.28±0.01	53.28±0.02	41.28±0.01	32.18±0.01	16.22±0.02
Cr	4.61±0.01	4.02±0.03	3.84±0.04	1.82±0.03	4.28±0.01	3.84±0.04	2.98±0.04	1.20±0.05	4.24±0.02	3.84±0.04	2.54±0.02	1.24±0.05
Ni	4.29±0.02	2.62±0.02	0.76±0.01	0.07±0.01	2.92±0.02	1.62±0.02	0.82±0.01	0.071±0.01	2.82±0.01	1.58±0.03	0.76±0.01	0.68±0.03

Fig 1 Map showing the National Highway No. 4 passing between Jamkhandi to Mudhol



Roadside soil gave higher concentration of Cu due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of cars derived from engine wear, brussing and bearing metals (Al-Khashman, 2007). The mean Cu level in roadside soil 49.98µg/g was found to be much higher the grass 4.87µg/g and ficus 4.70µg/g.

The source of zinc in relation to automobile traffic is wearing of break lining, looses of oil and cooling liquid (Saeedi et al., 2009). Arithematic mean of Zn of the roadside soil of around Jamkhandi shows a relatively high level of 188.8µg/g with a range of 34.20µg/g -398.02µg/g. The range of Zn 24.42 µg/g – 36.7µg/g found in ficus and grass 24.48 µg/g – 34.16µg/g (roadside) is not much higher. This can be attributed to the fact that Zn as an essential element is normally in uncontaminated plants up to 100 µg/g (Ho and Tai, 1988).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process , thus, plants can easily absorbs Cd from soil and transport to the shoot system.

Cadmium induces complex changes in plants genetically, biochemical and physiological levels. Our analysis for Cd in the roadside plants and control area. Cadmium level in the roadside soil averaged about 2.4µg/g and was the lowest among the seven metals examined. The mean Cd in ficus 1.42µg/g and in grass 1.594µg/g. Our finding are in confirmation with findings of (Ho and Tai, 1988).

The soil, grass and ficus contained much higher levels of Mn than other metals examined. Roadside soil, grass and ficus had average 1542µg/g, 56.804µg/m and 56.10µg/g of Mn content of the roadside soil may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil. Chromium is considered as a serious pollutant due to wide industrial use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are determined to their growth and development. Significant differences in our analysis for Cr in soil and in plant samples are found. Chromium level too was very high in roadside soil (326.5µg/g) against the control value of 124.42µg/g. In grass it was 4.89µg/g and in ficus it was found to be 4.62µg/g against control (Zero). Nickel level was considerable and was in roadside soil (88.98 µg/g) against control value (71.0 µg/g). In grass it was 10.94µg/g and in ficus, it was found that 9.12µg/g against control (7.16µg/g).

Simple linear regression between the metals viz, Pb, Cu, Ni, Mn, Zn, Cd and Cr present in the soil, grass and ficus were calculated and are given in the Tables 3and 4.

According to simple linear regression between the metal levels in roadside soil and ficus were found in Zn, Cd and Ni are significant at 5% level ($P < 0.05$). It may be indicating the bio-

concentration of these metals in the ficus, in addition to aerial deposition. This may be attributed to the favourable root environment (Sahu and Warrier, 1985) i.e, soil conditions might have favored their absorption.

Simple linear regression in case of chromium, nickel, manganese and copper contents between the soil, grass and ficus are not significant at 5% level, were low due to low bioavailability of these metals owing to unfavorable root environment. Whatever excess content of these metals found in soil, grass and ficus was pressured to be due to aerial deposition contributed by motor vehicles and other anthropogenic activities.

The order of increment of heavy metals in roadside is as follows

Soil: Mn > Cr > Zn > Pb > Ni > Cu > Cd
Grass: Mn > Zn > Pb > Ni > Cr > Cu > Cd and
Ficus: Mn > Zn > Pb > Ni > Cu > Cr > Cd.

The elevated levels of heavy metals in the road side soil and ficus is an indication of airborne pollutants of road side environment of the urban area of Jamkhandi city and along the road soil has high retention capacity for the heavy metals (Yassoglou, et al., 1987) due to there cation exchange capacity (CFC), complexing organic substances, oxides and carbonates. Thus, contamination levels increase continuously as long as the nearby sources remain active. During the last two decades, the city of Jamkhandi to the extent has witnessed sharp increase in vehicle number due to urbanization. Similar observation in Neem and Caesalpinia in mudhurai city of southern region of Tamil Nadu (Thambavani and Vanthana, 2013) .

In soil, the lesser mobility of metals and its accumulation on a long term basis, leads to overall higher contamination level of metals, Whereas, in roadside grass, ficus represents more accumulation due to turnover of plant materials (like new growths, the senescence followed by the abscission of old parts) and meterological influence (Kabata-Pendias, 2005). Thus , the study of metal concentration of roadside soil, grass and ficus reflects the extent of aerial contamination of roadside environment. The penetration of heavy metals into the food chains due to vehicular emissions may cause a long-range ecological and health hazard.

Accumulation profile of heavy metals in Crops

There are significant differences between the distribution of heavy metals in the crops at different Sampling station with varying distances (Table. 5). The accumulation of heavy metals was found to be high in all test crops at different locations compare to control and found in the order of 5 mt > 25mt > 50mt > 1000mt (control). The mean concentration of Pb level in test sugarcane collected from 5 to 50mt from the edge of road was recorded as 22.72 ± 1.81µg/g to 8.12 ± 0.03µg/g in maize it was recorded as 18.21 ± 0.03 µg/g to 4.26 ±0.02µg/g and in wheat it was recorded as 15.72 ± 0.02 µg/g to 3.27 ± 0.07µg/g, which was significantly higher than Indian standard (2.5µg/g) recommended by Awasthi, (2000). The permissible tolerable limit in agricultural crops is 10.0 µg/g and normal is varying from 5.0 to 15.0µg/g (Kabuta-Pendias 2005).

Lead is a poisonous metal, in human it is directly absorbed in to blood stream and is stored soft tissues, bones and teeth. Due to bioaccumulation it leads to chronic damage to central nervous system (CNS) and peripheral nervous system (PNS) and also brings difficulties in pregnancy (Peokjoo et al., 2008). It includes aberrant gene transcription (Boutan et al., 2001)

The mean concentration of Cu level in test sugar cane collected from 5 to 50mt from the edge of the road was recorded as 4.93 ± 0.02 µg/g to 3.04 ± 0.02 µg/g, in maize it was recorded as 4.94 ± 0.02 µg/g to 3.82 ± 0.01 µg/g and also in wheat it was recorded 4.82 ± 0.07 µg/g to 3.92 ± 0.01 µg/g which was significantly lower than tolerable limit in agricultural crops for Cu is 50µg/g and normal limit is about 5-30µg/g (Kabuta-Pendias 2005) copper is essential element but higher concentration intake leads to severe mucosal irritation, widespread capillary damage (Salmeron and Pozo, 1989).

The tolerable limit of agricultural crops for Zinc is 300 µg/g and normal is 27-150µg/g. The mean concentration of Zinc level in sugarcane collected from 5 to 50 mt from the edge of the road was recorded as 32.81 ± 0.01µg/g to 22.04 ± 0.03 µg/g, in maize recorded as 30.98 ± 0.02µg/g to 16.02 ± 0.04µg/g and also in wheat it was 31.04 ± 0.02 µg/g to 18.42 ± 0.04 µg/g respectively.

Zinc is considered to be relatively nontoxic, however, excess amount can cause system dysfunctions that results in impairment of growth and reproduction (Dubey et al., 2007). Excess concentration of metal in the body bound in various transcription regions such as polymerase enzymes (Wang et al., 1997).

Manganese is micronutrient , essential for physiological functions. The tolerable limit for Mn in agricultural crops is 300µg/g and normal value is 30 to 300 µg/g (Kabuta-Pendias 2005). The mean concentration of Mn level in sugarcane collected from 5 to 50 mt from the edge of rod was recorded as 50.12 ± 0.01 µg/g to 28.12 ± 0.04 µg/g, in maize it was recorded as 52.08 ± 0.02 µg/g to 36.28 ± 0.02 µg/g and also in wheat it was recorded as 53.28 ± 0.02 µg/g to 32.18 ± 0.01 µg/g respectively. Mn concentrations in test crops lower than upper limit recommended by Kabuta-Pendias (2005). But higher concentration is toxic causing neuropscychiatic disorder characterized by irritability, difficulty in Walking and Speech disturbances (Singh and Kalmadhad, 2011).

The permissible tolerable limit in agricultural crops for Cd is 3.0 µg/g and normal is varying from 0.05 to 0.2 µg/g (Kabuta-Pendias 2005).In control (1000mt) crop plants maximum accumulation is recorded in sugar (0.88 ± 0.01µg/g) and minimum is 0.64 ± 0.06µg/g in wheat.

Cadmium accumulate in the human kidney, respiratory system, cardiac failure and is also associated with bone diseases (Singh and Kalamdhad-2011). (Wang and Crowley 2005) also reported that discruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of Cd-toxicity Cd level in sugar collected from 5 to 50 mt from the edge of the road was recorded as 1.54 ± 0.02 µg/g to 1.02 ± 0.04 µg/g, in maize it was recorded as 1.64 ± 0.01 µg/g to 0.86 ± 0.01µg/g and also it was recorded to about 1.32 ± 0.03 µg/g to 0.88 ± 0.04µg/g in wheat respectively.

Chromium is considered as a serious environmental pollutant, due to industrial (wide) use (Shanker et al., 2005). Chromium compounds are highly toxic to plants and are detrimental to their growth. The mean concentration of Cr level in sugarcane

collected from 5 to 50 mt from the edge of road was recorded as 4.61±0.01 µg/g to 3.84±0.04 µg/g; in maize it was recorded as 4.28 ± 0.01 µg/g to 2.98 ± 0.04 µg/g and also in wheat to about 4.24 ± 0.02 µg/g to 2.54 ± 0.02 µg/g respectively.

Nickel has been considered to be an trace essential trace element for human (Animal) health (Zhuang et al., 2012). The permissible tolerable limit in agricultural crops is 50µg/g and normal is about 0.1 to 5.0µg/g. The mean concentration of Ni level in sugarcane collected from 5 to 50 mt from the edge of road was recorded as 4.29 ± 0.02 µg/g to 0.76 ± 0.01µg/g, in maize it was 2.92 ± 0.02 µg/g to 0.82 ± 0.01 µg/g and also in wheat it was 2.82 ± 0.01 µg/g to 0.76 ± 0.01 µg/g respectively. Nickel occurs mainly in the form of Sulphide and silicate minerals. Ni when administrated to animals is rapidly distributed to kidneys, pituitary, lungs, skin, adrinals, ovaries and testis (Sundarman-1989). Ni is carcinogenic to human and risks are highest for lung and nasal cancers. Ni also damages DNA directly through reactive oxygen species (McCoy and Kinney,1992).

CONCLUSION

Based in the analysis and results, it could be concluded that study on roadside soil, test plants and crops confirmed that vehicular emission is potential source of environmental pollution. The high level concentration Lead, Cadmium and Nickel concentration in soil will affect the health of the residents as well as surrounding communities, which may also affect soil fertility too. The consumption of these crops can considered safe with no risk to human health. The average intake of metals in long time low level body accumulation of heavy metals and detrimental impact becomes apparent only several year of exposure. These findings also suggest that special attention should be taken to this traffic related environmental issue and further suggest that serious affords required to reduced the high level of soil remediation and before the consumption of crops/vegetables should washed to remove significant amount of aerial accumulation from the surface of crops/vegetables. Finally, it is recommended that economical plant (vegetable/crops) should not be cultivated along the roadside and especially in high traffic density areas.

Acknowledgement

The authors are thankful to the Principal, B.L.D.E.A's Com.BHS Arts and TGP Science College, Jamkhandi (Karnataka), Principal, B.V.V. Snaghas, Basaveshwar Science College Bagalkot (Karnataka), Chairman, PG Department Botany, Karnataka University, Dharawad (Karnataka) for providing necessary facilities to carry out research work.

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INTERNATIONAL JOURNAL OF RESEARCH CULTURE SOCIETY ISSN: 2456-6683 Volume - 4, Issue - 10, Oct – 2020
Monthly, Peer-Reviewed, Refereed, Indexed Journal Scientific Journal Impact Factor: 5.743
Received on : 30/09/2020 Accepted on : 14/10/2020 Publication Date: 31/10/2020

The value of creativity and innovation for entrepreneurs

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Abstract: *In ever changing modern world customer expect new goods and services. Therefore, successful entrepreneurs should come up with new ideas to solve the problems faced by people. Entrepreneurs are always engaged in value addition and deliver the superior quality goods services at cheaper prices. Business people always think in terms of new ideas to deliver superior goods at lowest possible cost by constantly improving the quality of goods/ services. New Ideas and thinking in a different way leads to new goods and services. Such new goods services help entrepreneurs to survive for the long term, to compete and to grow in the market.*

Keywords: *creativity, innovation, innovative corporations, corporations that failed to innovate, techniques and methods of creativity.*

1. INTRODUCTION:

The Creativity is the action of turning new and imaginative ideas into reality one. In the simple terms, it is characterized by the ability to perceive the world in the different ways, to find hidden patterns, and to generate solutions to the various businesses problems.

Now are days no business can be survived without introducing new things. Therefore, creativity is a spark of an idea that a business leader needs to achieve their goals. Creative thinking is all about thinking in a different way to get the better result. As per the research, business leaders always think about new ideas and therefore they likely going to be more successful.

2. Statement of Problems :

The concept of innovation and creativity consists of a combination of knowledge and skills that are used together to create new solutions to the various business problems. It is necessary to know that innovation is not only driven by technology. On the contrary, it is driven and applied in various sectors such as leadership, social change and business. Nowadays, maximum of the countries are not able enough to create the right environment which helps to encourages a best innovation ecosystem. Some countries are good in rank while other are to be not more innovative. Therefore, it is crucial to support innovation in developing countries.

In fact, entrepreneurship comes with a host of lots of challenges. Only experienced entrepreneurs have to deal with this no matter how long they have been into the business, trying to establish their own brand, adjust to match or exceed the competition and keep your business profitable is a challenge no matter how many years you have been into business.

But for first generation entrepreneurs, there are few unique challenges that are especially difficult to face. If you're just getting into them, or you're thinking about becoming a successful entrepreneur, be prepared for these significant hurdles.

3. Objectives of the study:

- To know how creativity and innovation is important for the survival of the organization.
- To understand how to analysis and exploit the opportunities.
- To gain capacity to give best possible solutions to the business problems.
- To mobilize available resources and allocate them to a commercial gain from the opportunities identified.
- To posses the knowledge, ingenuity, diligence, persistence and commitment to innovation.
- To know method and techniques and methods of developing creativity and innovation

4. Creativity:

In simple terms, Creativity refers to generate or recognize ideas, alternatives, or possibilities that may be useful in solving problems and also helps in communicating with others.

According to Harvard's Tedd Leavitt "creativity is thinking on new things and thinking in a new and different way on old problems".

According to leadership expert Warren Benn is "Today’s Successful entrepreneurs live and die according to the quality of their ideas".

Today we are living in a thinker's world. It means the logical Thinkers will do well in these days. Every idea is a product of Thinking and we must know that all products are the manifestation of idea naked in a thinkers mind. There are few people who see problems as their opportunities to improve and do something new or something better. Therefore, we may think to improve productivity and efficiency, achieve speed, enhanced comfort and convenience. Thinking in a new way can produce various alternatives and these alternatives can result in cheap and best goods /services. Therefore, thinking is a must in the life of all successful entrepreneurs.

4.1 Forms of creativity

1) We may think on manufacture of few more products with the help of maize. At present more than 50 goods are being manufactured
2) We may think on manufacturing a mobile which will be charged automatically with the solar power.
3) We may include a comb and scale in a pen.
4) We may think on fuel efficient cars and bikes.
5) We may think on most attractive motor car & bikes.
6) We may think on flying car or driverless car.
7) We may think on use of robots in farms and factories.
8) We may think on generating electricity from gyms otherwise the energy becomes a waste.
9) Doctors and scientist may think on getting a child of desired qualities and so on

5. Innovation:

Creativity is thinking function but, innovation is doing function. Innovation is concerned with converting the dreams (Creativity) into reality. Innovation gives a concrete shape to creative thinking.

It is the process of brining the best ideas into value. We can't innovate without creativity. Innovation combines ideas and knowledge into goods and services. Without innovation an enterprise's goods/services becomes obsolete. It is doing new things or doing old things in a new way. It is an act of adding the value so as to have customers delight. Therefore, the main object of innovation is to pass more benefits, satisfaction. Delight to customers. Innovation is an essential prerequisite of a successfully entrepreneur. Innovation may arise out of information gathered from new connections: information gained from journey into other places. Innovation arises from organizing circles of exchange, where information is not only stored but, also created. It is a systematic effort to change and improve the quality of goods/services that are manufactured and sold to customers. It requires a fresh way of looking at things/ services. An undertaking of people and willingness to take risks and to work hard, merely new idea doesn't become an innovation unless it is widely accepted by people. Many people may resist for a change. But the innovation convinces such people by taking them into confidence. It is because of innovations we are able to find new and improved goods / services in the market.

Innovation may be defined "as changes made by the entrepreneur in factors production may be in the form of land, labor, capital and organization

It may also be defined "as a systematic improvement in the method of production. It refers to doing of new things or doing of things that are already being done in a new way'. It may take the form of a new product/service, a new technology or a new market or a new source of raw materials or new and improved organization.

The National Innovation Initiative defines as "The inter-section of invention and insight, leading to the creative of social and economic value".

5.1 It may take the following forms:

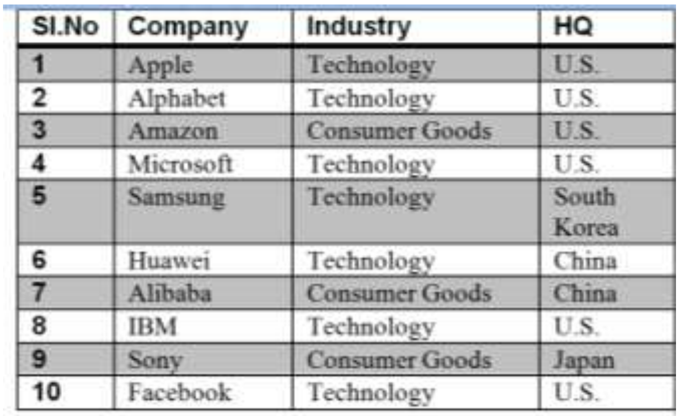
a) The development of a new product/ service in the market.
b) Introduction of new and improved technology which is not yet tested by others.
c) Finding a new market (people) i.e. searching for new buyers either to untapped.
d) The discovery of a new source of supply of raw material. It may be finding of alternate or substitute or cheap raw material.
e) Establishing a new form of organizing business so as to reduce the costs and enhance the managerial efficiency. It may result in formation or breaking up of monopoly

6. Name of the corporations that failed to innovate:

In this case, we can see so many famous corporations that suffered from innovation failure, including companies that have gone out of business. These are most reputed companies. In fact they are not examples of companies that are not innovative, but there is mixture of some failures. Let us to have some examples in below image that got failure due to innovation.

7. Most innovative corporations :

In the today's fast faced world, in order to have success companies need to adopt quickly changing market and shifting consumer behaviors. Here we can see the most innovative companies in 2020 based on **1.** Votes of Innovation Executives. **2.** Total Share Return **3.** Industry Disruption **4.** Industry Peer Review



Sl.No	Company	Industry	HQ
1	Apple	Technology	U.S.
2	Alphabet	Technology	U.S.
3	Amazon	Consumer Goods	U.S.
4	Microsoft	Technology	U.S.
5	Samsung	Technology	South Korea
6	Huawei	Technology	China
7	Alibaba	Consumer Goods	China
8	IBM	Technology	U.S.
9	Sony	Consumer Goods	Japan
10	Facebook	Technology	U.S.

8. Techniques and methods of developing Creativity and innovations:

Entrepreneurs are to give top priority to development of creative ideas and innovations to survival and grow in the market. Creativity plays pivotal role in maximizing sales and profits. Business should always dance according to the dream beaten by customers. Creativity and innovations can be developed by following techniques.

- **Suggestions Box:** In this case, employees, customers, entrepreneurs are to be motivated to come up with new ideas, preferably new best ideas should be rewarded. There must be suggestion box must be kept in the office premises. People should be requested to drop their new innovative ideas in the suggestion box by keeping them in the most prominent places in the business premises by opening them on regular interval.
- **Brain-storming session:** it is an arrangement to collect new ideas from a specific group of people. It is most popular and oldest technique of collecting ideas in respect of goods and services.
- **Universities and research labs:** Research activities are conducted by universities and laboratories. An entrepreneur should keep constant contact with such agencies. It helps him in gathering useful information in connection with updating technology. New products, new services, new method of organizing business or new method of marketing of goods/services.
- **Reverse Brain-storming**: In this technique, workers are requested to express their new and navel ideas about brand new products and services
- **Initiative technique:** Initiative refers to freedom to propose a new plan and to implement it. Entrepreneur should give sufficient freedom to his assistants to propose new ideas. Workers are in touch with the problems and developments
- **Reversal technique:** This technique is commonly used to improve the quality of goods/services. Reversal technique asks negative questions to get creative ideas. for example,: How not to increase the profits?
- **Mind mapping:** it is a technique of logical thinking. It is a graphical representation which encourages thinking in a different way. This method uses to write a problem or picture

- **Provocation:** It is a technique of collecting new and breaking ideas from respondents. Here peoples mind is provoked by making challenges.
- **Simplex:** This technique treats the creativity as a cycle and it is continuous. This cycle generates new ideas by throwing light.
- **Inviting creative ideas from mass**: in this method, business men invite people (customers) in news paper, magazines, internet, television etc. A clear cut problem is given with a request to come up with new ideas. Selected ideas are suitably rewarded.

9. CONCLUSION:

Creativity and innovation play a vital role in exploring the new market opportunities, getting the success in the area of every business through higher degree of efficiency, increased productivity and better quality etc.

To be successful entrepreneur requires focusing on creativity and integration of innovation and other strategic business practices.

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Journal of Advancements in Library Sciences
ISSN: 2349-4352
Volume 7, Issue 1
www.stmjournals.com

Modelling The Growth of Chemistry Literature from 2005-2016: A Scientometric Study

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Abstract

The present study demonstrates the growth of Chemistry literature for the period 2005-2016. A total of 24322 records were extracted from the Scopus Database for twelve years which is used as main source of primary data for the present study. The growth models were applied for the literature of Chemistry. The result of the study indicates that, the Relative Growth Rate (RGR) of Chemistry publication found to be decreasing trend and Doubling Time (Dt) found to be increasing trend. The growth of literature in the field of Chemistry does not follow either Polynomial or Power growth model. The study concluded that there has consistent trend in the growth of Chemistry literature. The study can be concluded that chemical literature follows the moderately follows Linear growth, Exponential growth and Logistic growth model.

Keywords: *Scientometrics, Chemistry Literature, Relative Growth rate (RGR), Doubling Time (Dt), Growth Models*

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INTRODUCTION

One of the features of modern research in recent years has been the spectacular development of scientific discoveries and growth of knowledge, say Gupta et al. (2002) [1]. This has caused an unprecedented accumulation of information and has become a major concern for scientists and researchers [2].

Scientometric, is one of the quantitative tools which is developed in 21st century in library and information science, it can be applied to any discipline irrespective of their period of evaluation and quantitative studies of scientific studies. The assessment of research performance using Scientometric techniques is a valuable method for the identification and evaluation of the strengths and weaknesses in scientific achievements. The generation of new Knowledge/Information has been accelerating over the past several years in the field of scientific and technical. In recent years increasing attention has been paid to the social dimensions of scientific community that produces sciences. But this unprecedented growth in literature has become a major concern for the scientists, scholars, and library professional as they try to keep themselves abreast with new advances in their subject and information professionals try to organize this knowledge. Growth of literature reflects in various national level activities in Research & Development, institution a matters of great concern to the managers of scientific activities in government industry and in academic community. This kind of growth study will be of practical value to the chemical scientist, library professionals and policy makers in effective management of the action.

REVIEW OF LITERATURE

Mahapatra (1994). Discussed the relative growth rate (RGR) and doubling time (Dt) for publications and citations which appeared in Indian library and information science journals during 1975 to 1985 were determined [3]. The reducing trend of RGR and increasing rare for doubling time in both-publications and citations indicates that the growth is neither exponential nor linear. The size of the literature is calculated by applying logistic growth formula. Publication on different disciplines follows the similar type of growth trend within equal economic, intellectual and environmental conditions and with the increase of number of publications, the number of citations will also increase.

Seetharam and Ravichandra Rao (1999) have made an attempt to compare the trends in the growth of Food Science and Technology (FST) literature published by CFTRI scientists, in India, and food scientists of the world, the study covers from 1989 to 2013. Finally, the authors identify the best fitting growth models for actual and cumulative growth of data through various growth models [4]. Different approaches are introduced by Gupta and Karisiddappa (2000) in their paper for studying the growth of scientific knowledge as reflected through publications and authors [5].

Neelamma G and Gavisiddappa Anandhalli (2015) The study identifies the various parameters of crystallography literature like year wise distribution, relative growth rate, doubling time of the literature, geographical wise, organization type, Language wise, document wise, most productive authors and funding institutions etc [6]. Most articleswere published in the year of 2011, while less numbers of research articles were reported in the year 1999. Further, the relative growth rate is gradually increasing and on the other hand doubling time decreases. Large majority of the research publications are published in English version andmajority of them published in the form of research articles. China published highest number of research articles in the area of Crystallography.

Hadagali Gururaj and Anandhalli (2015) The study indicates that the growth of literature in neurology literature does not follow the linear or logistic model [7]. But it follows closely the exponential growth model, the study reveals that there has been a consistent positive trend towards increased growth of literature in the field of neurology.

Neelamma and Anandhalli (2016) The study depicts on various bibliometric tool such as distribution of citations by publication type, Country wise publication of citations, further the study author also identify the core journals in the field of crystallography [8]. The analysis of the study reveals that out of 1387195 citations which (83.835%) Research articles contribute the highest number of citations and it is the most preferred sources of information used by researcher in the area of crystallography. Further it is observed that Journal of Molecular Biology is one of the highly cited journals in the field of chemistry and its allied subject. Highest research publications were reported from the USA in the world. Bradford’s law well followed and tested for the given data set. Finally, it can be summarised that, the lot of research activity is being taking place in the field of Crystallography and it is emerging one of the leading subjectsin the applied sciences [9].

METHODOLOGY

The dataset was collected from the SCOPUS database for the period 2005-2016 in the field of chemistry. A total of 24322records were retrieved for the period of twelve years. For the present SCOPUS database is considered as main source of data, it is one of the most comprehensive databases covering all subjects especially in the field of science and technology. Majority of the chemistry research output is indexed in Scopus database hence, for the present study Scopus is considered. The keywords ‘Chemistry’ and their combination of words within string have been used for extracting the number of records available in the said database. The retrieved records were processed, classified, and analysed based on the objectives of the study. Further, the data is analysed using MS Excel spreadsheet and SPSS software to draw the meaningful conclusion for the study.

OBJECTIVES OF THE STUDY

The specific objectives of the study

1. To study the year wise distribution and average growth of literature in the field of Chemistry literature.
2. To examine the relative growth rate and doubling of the literature in the field of chemistry as reflected in the SCOPUS.
3. To analyse the fit of Chemistry literature in terms of different growth models.

Hypothesis

The growth publication in the field of chemistry literature follows the linear growth/ exponential/ logistic growth model.

DATA ANALYSIS AND INTERPRETATION

Table 1 depicts the year wise contribution and average growth rate of articles in the Chemistry literature from 2005-2016. It is evident from the table-1 that 24322 articles were published during the study period (2005-2016). It is observed that highest numbers of articles (N=2094, 8.61%) were recorded in the year 2016. The second highest number of articles (N=2032, 8.35%) were observed in the year 2015, while lowest number of articles were contributed in the year 2008 (N=2006, 8.25%). Further, it is found that the average growth rate of the articles is found to be 0.996. It has been observed that number of articles increase gradually from 2005-2016 (Figure 1).

Further descriptive statistics of articles shows that the average growth rates of articles found to be 0.996 and on an average 24322 articles were published in each year during the study period with a variation of 22.65 articles over a period of twelve years. The highest number of articles i.e. 2094 were published in the year 2016. During the study period and lowest number of 2006 were published in the year 2008.

Table 1: *Year Wise Growth Rate of World Chemical Literature from 2005-2016.*

SI. No.	Year	No of article	% age	Cum	Cum %age	Growth rate	Descriptive Statistics	
1	2005	2010	8.26	2010	8.26		Average Growth	0.996
2	2006	2016	8.29	4026	16.55	0.997	Mean	2026.83
3	2007	2024	8.32	6050	24.87	0.996	SD	22.65
4	2008	2006	8.25	8056	33.12	1.009	MAX	2094.00
5	2009	2030	8.35	10086	41.47	0.988	MIN	2006.00
6	2010	2015	8.28	12101	49.75	1.007	Range	1.04
7	2011	2020	8.31	14121	58.06	0.998		
8	2012	2021	8.31	16142	66.37	1.000		
9	2013	2031	8.35	18173	74.72	0.995		
10	2014	2023	8.32	20196	83.04	1.004		
11	2015	2032	8.35	22228	91.39	0.996		
12	2016	2094	8.61	24322	100.00	0.970		
		24322	**100**			**0.996**		

Fig. 1: *Year wise Growth of Articles.*

(a) Relative Growth Rate (RGR)

RGR is the growth rate publication related to the size of publication. It is also known as the exponential growth rate or continuous growth rate with reference to scientific literature publication. RGR means the increase in the number of articles per unit of time. Further the mean of RGR of articles over specific period can be calculated by using the formula:

$$R = \frac{W_2 - W_1}{T_2 - T_1}$$

Where:

R= Relative Growth Rate of Articles over specific period of time

W_2= Log W2 (Natural log of final number of publications)

W_1= Log W1 (Natural log of initial number of publications)

T_2= Final Time in Years

T_1= Initial Time in Years

This formula still holds good for the calculations of RGR subject wise.

(b) Double Time (Dt)

The doubling time is the given period required for quantity to double in size or value. It is concerned with RGR, where RGR is constant. The quantity undergoes exponential growth and has a constant doubling time or period which can be calculated directly from growth rate. This can be calculated by using the formula.

$$Dt(P) = \frac{Loge^2}{R(P)} = \frac{0.693}{R(P)}$$

Dt(P)= Average doubling time of publications

***Table 2:** Relative Growth Rate (RGR) and Doubling Time (Dt) of Articles in Chemical Science from 2005 to 2016.*

SI.No	Year	Quantum of output	Cumulative output	W1	W2	Rt(p)	Mean RP(p)	Dt(p)	Mean Dt(p)
1	2005	2010	2010	0.00	7.61	0.00	0.36	0.00	2.40
2	2006	2016	4026	7.61	8.30	0.69		1.00	
3	2007	2024	6050	7.61	8.71	0.41		1.70	
4	2008	2006	8056	7.60	8.99	0.29		2.42	
5	2009	2030	10086	7.62	9.22	0.22		3.08	
6	2010	2015	12101	7.61	9.40	0.18		3.80	
7	2011	2020	14121	7.61	9.56	0.15	0.12	4.49	6.17
8	2012	2021	16142	7.61	9.69	0.13		5.18	
9	2013	2031	18173	7.62	9.81	0.12		5.85	
10	2014	2023	20196	7.61	9.91	0.11		6.57	
11	2015	2032	22228	7.62	10.01	0.10		7.23	
12	2016	2094	24322	7.65	10.10	0.09		7.70	
		24322							

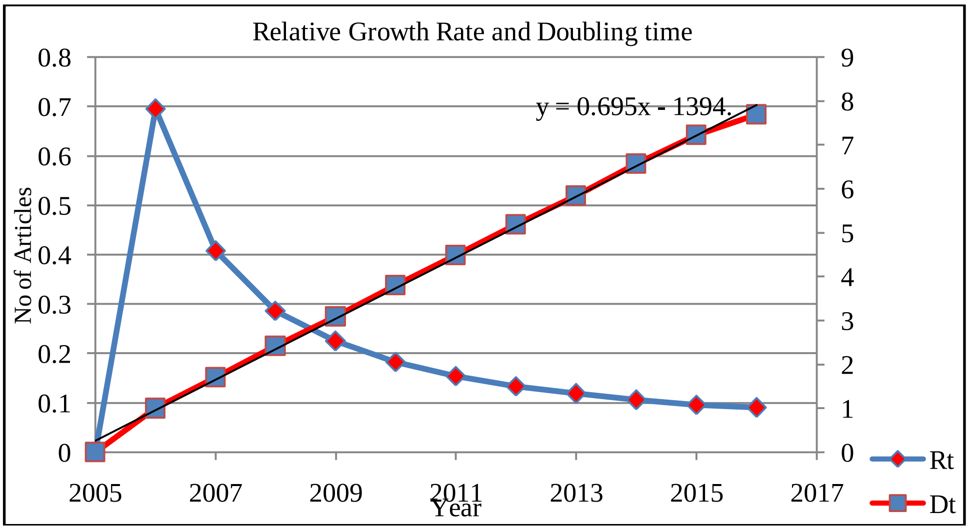

***Fig. 2:** Relative Growth Rate (RGR) and Doubling Time (Dt).*

Table 2 shows the Chemical literature contributions i.e. 24322 articles. The average relative growth rate of articles of contribution has come down from 0.69 (2005) to 0.09 (2016) over a period of twelve years. The mean relative growth for the first six years (2005 to 2010) exhibits a growth of 0.36. Similarly, for the next block of six years (2011 to 2016) the growth is 0.12.

At the same time, doubling time of publication of articles increased gradually over a period from 1.00 in the year 2005 to 7.70 in the year 2016 of twelve years. Simultaneously, the value of Doubling time (Dt) increased in the first block period of six years is 2.40 (2005-2010). While, in the second block period, the doubling time (Dt) increased from 6.17 in the year 2011 to 2016 (Figure 2).

(c) Linear growth model
The linear growth model is describing growth to be constant or similar from year to year, thus a graphic representation of the yearly data accumulated would be a straight line.

Hypothesis-3
The growth publication in the field of chemistry literature follows the linear growth.
Testing of hypothesis
To find out the growth pattern in the field of chemistry literature, publication over the last twelve years (2005-2016) were considered as sample of data set for the present study of the analysis in order to fit the data to test whether the growth of literature in chemistry follows the linear growth pattern or not (Table 3). The expected numbers of publications (y) or (p) were computed suing the following formula
Y1=ax+b

Where a and b are constant
X is the unit of time

Inferences:
The results of chi-square test of goodness of fit indicated that the calculated Chi- Square value (1.65285) is less than the critical value of 19.38 for 11 degree of freedom (df) at .05 (5%) level of significance. Hence the null hypothesis -1 is accepted, it can be concluded that the growth of literature follows the linear growth model (Figure 3).

***Table 3:** Applicability of Linear Growth Model.*

x	year	no of records f	Y1=ax+b (p)	(f-p)	(f-p)^2	$\frac{(f-p)^2}{p}$
1	2005	2010	2004.1	5.9	35.17676	0.017553
2	2006	2016	2008.1	7.9	61.81104	0.03078
3	2007	2024	2012.2	11.8	139.0748	0.069116
4	2008	2006	2016.3	-10.3	105.5962	0.052372
5	2009	2030	2020.3	9.7	93.21902	0.04614
6	2010	2015	2024.4	-9.4	88.6234	0.043777
7	2011	2020	2028.5	-8.5	71.96129	0.035475
8	2012	2021	2032.6	-11.6	133.4487	0.065656
9	2013	2031	2036.6	-5.6	31.59564	0.015514
10	2014	2023	2040.7	-17.7	312.9361	0.153348
11	2015	2032	2044.8	-12.8	162.7921	0.079614
12	2016	2094	2048.8	45.2	2040.51	0.99594
					Total	**1.65285**

Calculated constantis
a=4.69, b= 2000
Calculated value = 1.65285

(d) Exponential growth model
The exponential growth model describes an unlimited exponential growth. This model does not only provide the rate of growth but also the rate at which the size of the literature double, and its doubling time. The exponential growth has been linked to compound interest

Hypothesis-4
The growth of publication in the field of chemistry literature follows the exponential growth model.
Testing of hypothesis
In order to fit the data to test whether the growth of literature in chemistry follows the exponential growth pattern or not (Table 4). The expected number of publications (y) or (p) was computed using the following formula.
$Y= K+ab^x$

Where a and b are constant
K is the asymptote of the upper limit and X is the unit of time
K=2000,
Y=.002

y=K*e.002*x (Exponent e= 2.718)
Calculated constant
K=2000, Y= .002
Calculated value = 1.602032

Inferences

The results of chi-square test of goodness of fit indicated that the calculated Chi- Square value (1.6602032) is less than the critical value of 19.38 for 11 degree of freedom (df) at .05 (5%) level of significance. Hence the null hypothesis -4 is accepted, it can be concluded that the growth of literature is follow the Exponential Growth Model (Figure 4).

Calculated constant
K=15.68, Y= 2000
Calculated value = 1.965939
Table value, 11 df and .05 level of significance =19.38

Inferences

The results of chi-square test of goodness of fit indicated that the calculated Chi- Square value (1965939) is less than the critical value of 19.38 for 11 degree of freedom (df) at .05 (5%) level of significance. Hence the null hypothesis -5 is accepted, it can be concluded that the growth of literature is follow the Logistic Growth Model (Figure 5).

Table 4: ***Applicability of Exponential Growth Model.***

x	**Year**	**No of Records**	**y=k*e.002*x**	**f-p**	**(f-p)2**	**(f-p)2/p**
1	2005	2010	2004.004	6.0	35.95697	0.017943
2	2006	2016	2008.015	8.0	63.75721	0.031751
3	2007	2024	2012.035	12.0	143.1655	0.071155
4	2008	2006	2016.062	-10.1	101.2539	0.050224
5	2009	2030	2020.098	9.9	98.04486	0.048535
6	2010	2015	2024.142	-9.1	83.57725	0.04129
7	2011	2020	2028.194	-8.2	67.14121	0.033104
8	2012	2021	2032.254	-11.3	126.6525	0.062321
9	2013	2031	2036.322	-5.3	28.32531	0.01391
10	2014	2023	2040.398	-17.4	302.706	0.148356
11	2015	2032	2044.483	-12.5	155.8229	0.076216
12	2016	2094	2048.576	45.4	2063.382	1.007228
					Total	**1.602032**

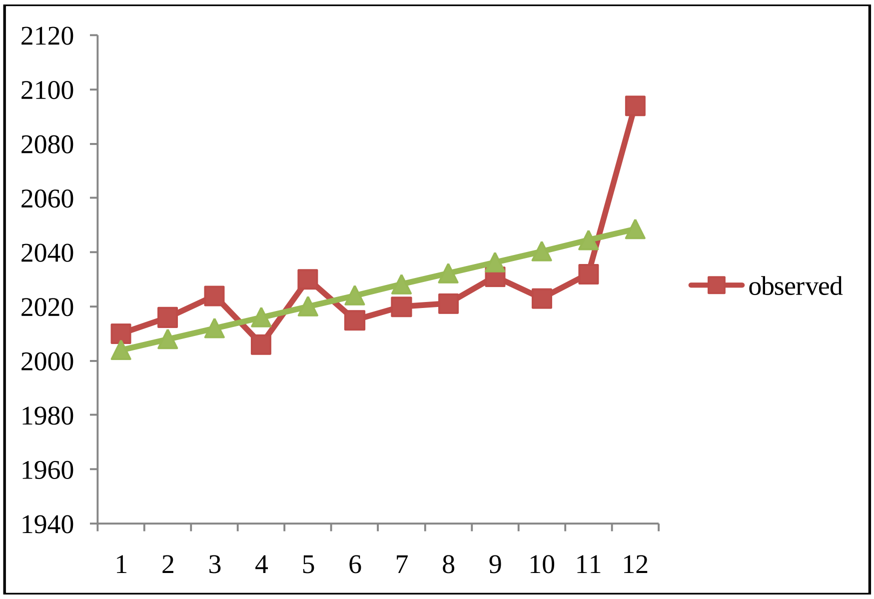

Fig. 3: *Degree of Freedom for Linear Growth Model.*

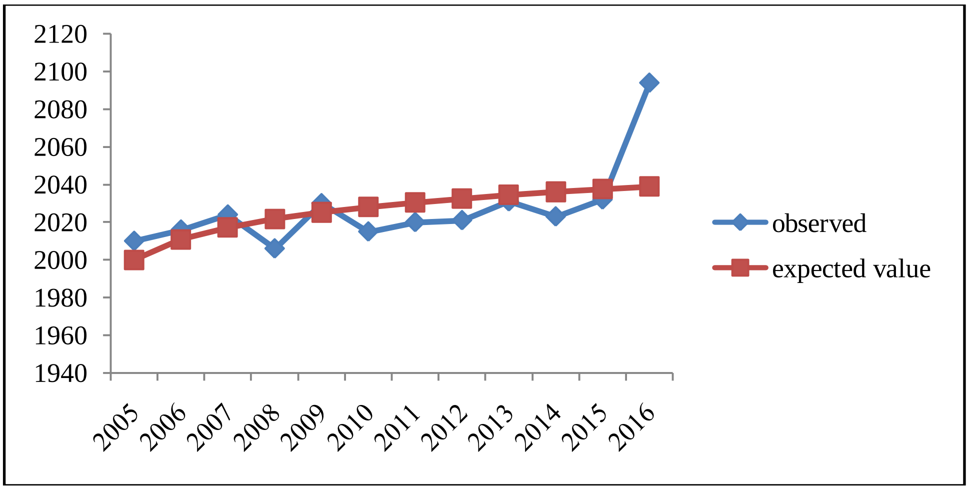

Fig. 4: *Exponential Growth Model (Number of Records and Number of Publication).*

Table 5: *Applicability of Logistic Growth Model.*

x	**year**	**no of records**	**y=15.68 *Ln(x)+2000**	**f-p**	**(f-p)2**	**(f-p)2/p**
1	2005	2010	2000	10.0	100	0.05
2	2006	2016	2010.869	5.1	26.3318	0.013095
3	2007	2024	2017.226	6.8	45.88382	0.022746
4	2008	2006	2021.737	-15.7	247.6562	0.122497
5	2009	2030	2025.236	4.8	22.69582	0.011207
6	2010	2015	2028.095	-13.1	171.4735	0.084549
7	2011	2020	2030.512	-10.5	110.4994	0.054419
8	2012	2021	2032.606	-11.6	134.691	0.066265
9	2013	2031	2034.452	-3.5	11.91963	0.005859
10	2014	2023	2036.105	-13.1	171.7288	0.084342
11	2015	2032	2037.599	-5.6	31.34878	0.015385
12	2016	2094	2038.963	55.0	3029.034	1.485576
					Total	**1.965939**

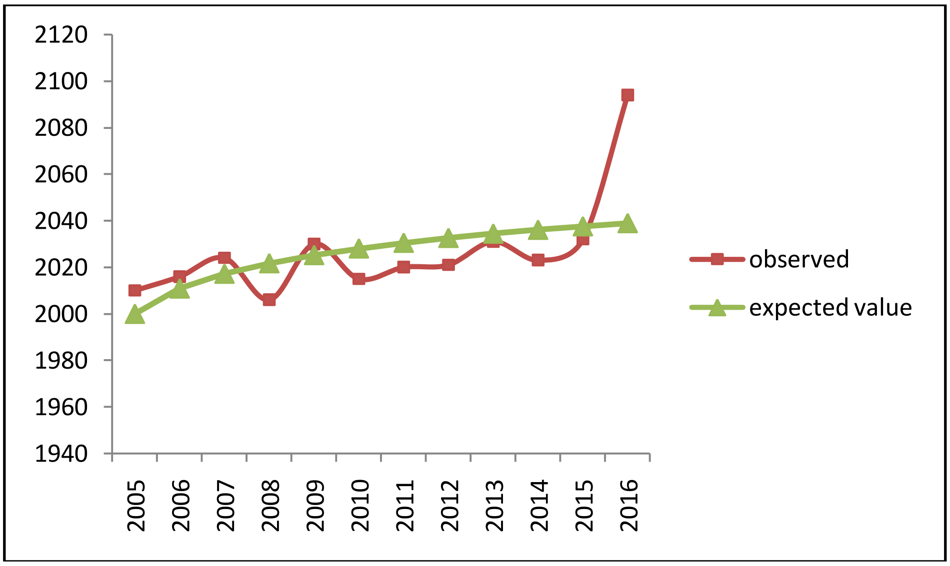

Fig. 5: *Year vs Number of Records in Logistic Growth Model.*

CONCLUSION

The study is based on 24322 research papers published between 2005-2016 as reflected in *Scopus Database*, which is one of the most comprehensive online databases covering all the subjects [10]. The data were collected, tabulated, and analysed. The study shows some factual factorial data through bibliometric analysis. Research articles have been analysed for finding the year wise trend, Relative Growth Rate, doubling time, and examining the different types of growth rate models By comparing the results obtained from actual statistical fits of the different growth models and the most appropriate growth model is likely to fit. The growth of literature in the field of Chemistry follows linear growth model. Exponential growth model and Logistic models. The study concluded that there has been a consistent trend towards increased growth of literature in the field of Chemistry [11,12].

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Cite this Article

Mahadevi R Nyamagoudar, Gavisiddappa Anandhalli. Modelling The Growth of Chemistry Literature from 2005-2016: A Scientometric Study. *Journal of Advancements in Library Sciences*. 2020; 7(1): 83–90p.

Electronic Journal of Mathematical Analysis and Applications
Vol. 8(1) Jan. 2020, pp. 75-99.
ISSN: 2090-729X(online)
http://math-frac.org/Journals/EJMAA/

M-POLYNOMIAL AND DEGREE-BASED TOPOLOGICAL INDICES OF GRAPHS

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Abstract. For a graph G, the *M-polynomial* is defined as $M(G;x,y) = \sum_{i\leq j} m_{ij}(G)x^i y^j$, where $m_{ij}, (i,j \geq 1)$, is the number of edges uv of G such that $d_G(u) = i$ and $d_G(v) = j$. The topological indices play an important role in determining *physico-chemical properties* of chemical graphs, among them the degree-based topological indices can be easily driven from an algebraic expression corresponding to the chemical graphs called *M-polynomial*. In this note, we first compute $M-$*polynomial* of some special graphs. Further, we derive some degree-based topological indices of these graphs from their respective $M-$*polynomial*.

1. Introduction

Throughout this paper, by a graph $G = (V,E)$ we mean a simple, undirected, finite graph of order n and size m. Let $V(G)$ and $E(G)$ denote the vertex set and an edge set, respectively. The *degree* $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident to it in G. Let $\{v_1, v_2, ..., v_n\}$ be the vertices of G and let $d_{v_i} = d_G(v_i)$. The *line graph* [13] $L(G)$ of a graph G is a graph whose vertex set is one-to-one correspondence with the edge set of the graph G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G. The *subdivision graph* [13] $S(G)$ of a graph G is the graph obtained by inserting a new vertex onto each edge of G. The *product* [9, 13] $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if and only if [$a = b$ and $xy \in E(H)$] or [$x = y$ and $ab \in E(G)$]. The *corona* [9, 13] $G \circ H$ of graphs G and H is a graph obtained from G and H by taking one copy of G and $|V(G)|$ copies of H and then joining by an edge each vertex of the i^{th} copy of H is named (H,i) with the i^{th} vertex of G. The *join* [13] $G_1 + G_2$ of two graphs G_1 and G_2 is the graph obtained from G_1 and G_2 by joining every vertex of G_1 to all vertices of G_2. For undefined graph theoretic terminologies and notions, refer to [13, 15, 23].

It is always interesting to find some properties of graphs which are invariant. Topological indices and polynomials are foremost among them. Over the last decade

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2010 *Mathematics Subject Classification.* 05C07, 05C31.

Key words and phrases. M-polynomial, degree-based topological indices, edge partitions, graph invariant.

Submitted March 27, 2019. Revised April 5, 2019.

there are numerous research papers devoted to topological indices and polynomials. Several topological indices have been defined in the literature. For details of topological indices one can refer to [7, 16]. For different topological indices and their applications one can refer to [1, 2, 3, 10, 11, 12]. The general form of degree-based topological index of a graph is given by

$$TI(G) = \sum_{e=uv \in E(G)} f(d_G(u), d_G(v))$$

where $f = f(x, y)$ is a function appropriately chosen for the computation. Table 1 gives the standard topological indices defined by $f(x, y)$.

There are many graph polynomials too [4, 25]. The Hosoya polynomial is the most well-known polynomial which plays a vital role in determining distance-based topological indices such as Wiener index [24], hyper Wiener index [4] of graphs. The $M-polynomial$ [5] is one among other algebraic polynomials which was introduced in 2015 and useful in determining many degree-based topological indices (listed in Table 1) [7, 16]. Recently, the study of $M-polynomial$ are reported in [18, 19, 20].

Definition 1. [5] *If G is a graph, then $M-polynomial$ of G is defined as*

$$M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j, \tag{1.1}$$

where $m_{ij}, (i, j \geq 1)$, is the number [6] of edges uv in G such that $d_G(u) = i$ and $d_G(v) = j$.

Table 1. Operations to Derive degree-based topological indices from $M-$polynomial [5].

Notation	Topological Index	$f(x,y)$	Derivation from $M(G;x,y)$
$M_1(G)$	First Zagreb	$x+y$	$(D_x + D_y)(M(G;x,y))\|_{x=y=1}$
$M_2(G)$	Second Zagreb	xy	$(D_x D_y)(M(G;x,y))\|_{x=y=1}$
$^mM_2(G)$	Second modified Zagreb	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y))\|_{x=y=1}$
$S_D(G)$	Symmetric division index	$\frac{x^2+y^2}{xy}$	$(D_x S_y + D_y S_x)(M(G;x,y))\|_{x=y=1}$
$H(G)$	Harmonic	$\frac{2}{x+y}$	$2S_x J(M(G;x,y))\|_{x=1}$
$I_n(G)$	Inverse sum index	$\frac{xy}{x+y}$	$S_x J D_x D_y(M(G;x,y))\|_{x=1}$

where $D_x = x\frac{\partial f(x,y)}{\partial x}$, $D_y = y\frac{\partial f(x,y)}{\partial y}$, $S_x = \int_0^x \frac{f(t,y)}{t}dt$, $S_y = \int_0^y \frac{f(x,t)}{t}dt$ and $J(f(x,y)) = f(x,x)$ are the operators.

2. M-polynomial of some special Graphs

Proposition 2.1. *The M-polynomial of a path, a cycle, a complete graph, a complete bipartite graph, a wheel, a star and a double star are as follows:*

(i) *For a path P_n of order n, we have*

$$M(P_n;x,y) = 2xy^2 + (n-3)x^2y^2.$$

(ii) *For a cycle C_n of order n, we have*

$$M(C_n;x,y) = nx^2y^2.$$

(iii) *For a complete graph of order n, we have*

$$M(K_n;x,y) = \binom{n}{2}x^{n-1}y^{n-1}.$$

(iv) *For a complete bipartite graph $K_{a,b}$ of order $a+b$, we have*

$$M(K_{a,b};x,y) = abx^ay^b.$$

(v) *For a wheel W_n of order $n+1$, we have*

$$M(W_n;x,y) = nx^3y^3 + nx^3y^n.$$

(vi) *For a star S_n of order $n+1$, we have*

$$M(S_n;x,y) = nxy^n.$$

(vii) *For a double star $S_{a,b}$ of order $a+b+2$, we have*

$$M(S_{a,b};x,y) = axy^{a+1} + bxy^{b+1} + x^{a+1}y^{b+1}.$$

Definition 2. *The vertex splitting graph [22] $S'(G)$ of a graph G is obtained from G by adding for each vertex v of G a new vertex v' so that v' is adjacent to every vertex that is adjacent to v.*

Theorem 2.2. *If G is a graph of order n and size m with the M-polynomial $M(G;x,y) = \sum\limits_{i\leq j} m_{ij}(G)x^iy^j$, then*

$$M(S'(G);x,y) = \sum_{i\leq j} m_{ij}(S'(G))x^iy^j = \sum_{i\leq j} m_{ij}(G)x^{2i}y^{2j} + \sum_{a\leq b} m_{ab}(G)x^ay^b,$$

where $m_{ab}(G) = \begin{cases} m_{ij}(G) & \text{for } a=i, b=2j \text{ and } i\neq j, \\ 2m_{ij}(G) & \text{for } a=i, b=2j \text{ and } i=j. \end{cases}$

Proof. By definition of vertex splitting graph, we have the degree of the original vertices of G in $S'(G)$ is twice the degree of that vertex in G while the degree of the duplicates of those vertices are the same as the degree of corresponding vertices in G. Therefore, we have the following:

$$m_{2i2j}(S'(G)) = m_{ij}(G) \text{ and } m_{ab}(G) = \begin{cases} m_{ij}(G) & \text{for } a=i, b=2j \text{ and } i\neq j, \\ 2m_{ij}(G) & \text{for } a=i, b=2j \text{ and } i=j. \end{cases}$$

Thus, we get the desired result by substituting these values in Eq. (1.1). □

Definition 3. *The edge splitting graph [14] $L_S(G)$ of a graph G is a graph with vertex set $E(G)\cup E_1(G)$ with two vertices adjacent if they correspond to adjacent edges of G or one corresponds to an element ${e_i}'$ of $E_1(G)$ and the other to an element e_j of $E(G)$ where $e_j \in N(e_i)$.*

Theorem 2.3. *If G is a graph of order n and size m with the M-polynomial $M(G;x,y)=\sum\limits_{i\leq j} m_{ij}(G)x^iy^j$, then*

$$M(L_S(G);x,y)=\sum_{i\leq j} m_{ij}(L_S(G))x^iy^j=\sum_{i\leq j} m_{ij}(L(G))x^{2i}y^{2j}+\sum_{a\leq b} m_{ab}(L(G))x^ay^b,$$

where $m_{ab}(L(G))=\begin{cases} m_{ij}(L(G)) & for\ a=i, b=2j\ \ and\ \ i\neq j,\\ 2m_{ij}(L(G)) & for\ a=i, b=2j\ \ and\ \ i=j.\end{cases}$

Proof. By definition of edge splitting graph, we have the degree of the original vertex of $L(G)$ in $L_S(G)$ is twice the degree of that edge vertex in $L(G)$ while the degree of the duplicates of those vertices are the same as the degree of corresponding vertices in $L(G)$. Therefore, we have the following:

$$m_{2i2j}(L_S(G))=m_{ij}(L(G))\ \ and\ \ m_{ab}(L(G))=\begin{cases} m_{ij}(L(G)) & for\ a=i, b=2j\ \ and\ \ i\neq j,\\ 2m_{ij}(L(G)) & for\ a=i, b=2j\ \ and\ \ i=j.\end{cases}$$

Thus, we get the desired result by substituting these values in Eq. (1.1). □

Definition 4. *The shadow graph [9] $D_2(G)$ of a connected graph G is constructed by taking two copies of G, say G', G'' and joining each vertex v' in G' to the neighbors of the corresponding vertex v'' in G''.*

Theorem 2.4. *If G is a graph of order n and $D_2(G)$ is the shadow graph of G, then*

$$M(D_2(G);x,y)=\sum_{i\leq j} 4m_{ij}(G)x^{2i}y^{2j}.$$

Proof. Let $D_2(G)$ be the shadow graph of a graph G of order n which has $2n$ vertices and $4m$ edges. Then we have by definition of shadow graph $d_{D_2(G)}(v')=2d_G(v)$ for each $v'\in V(D_2(G))$ corresponds to $v\in V(G)$. Thus,

$$\begin{aligned} |E_{\{2i,2j\}}| &= |uv\in E(D_2(G)) : d_u=2i\ \ and\ \ d_v=2i| \\ &= 2|u'v'\in E(G') : d_{u'}=i\ \ and\ \ d_{v'}=j|+2|u''v''\in E(G'') : d_{u''}=i\ \ and\ \ d_{v''}=j| \\ &= 2m_{ij}(G)+2m_{ij}(G) \\ &= 4m_{ij}(G). \end{aligned}$$

Thus, the $M-polynomial$ of $D_2(G)$ is

$$M(D_2(G);x,y)=\sum_{i\leq j} m_{ij}(D_2(G))x^iy^j=\sum_{i\leq j} 4m_{ij}(G)x^{2i}y^{2j}.$$

□

Corollary 2.5. *If G is an r-regular graph of order n and size m, then*

$$M(D_2(G);x,y)=4mx^{2r}y^{2r}$$

Definition 5. *For a graph $G=(V(G),E(G)$, the Mycielskian [21] $\mu(G)$ of G is a graph with vertex set consisting the disjoint union $V(G)\cup V'(G)\cup\{u\}$, where $V'(G)=\{x' : x\in V(G)\}$, and the edge set $E(G)\cup\{x'y : xy\in E(G)\}\cup\{x'u : x'\in V'(G)\}$.*

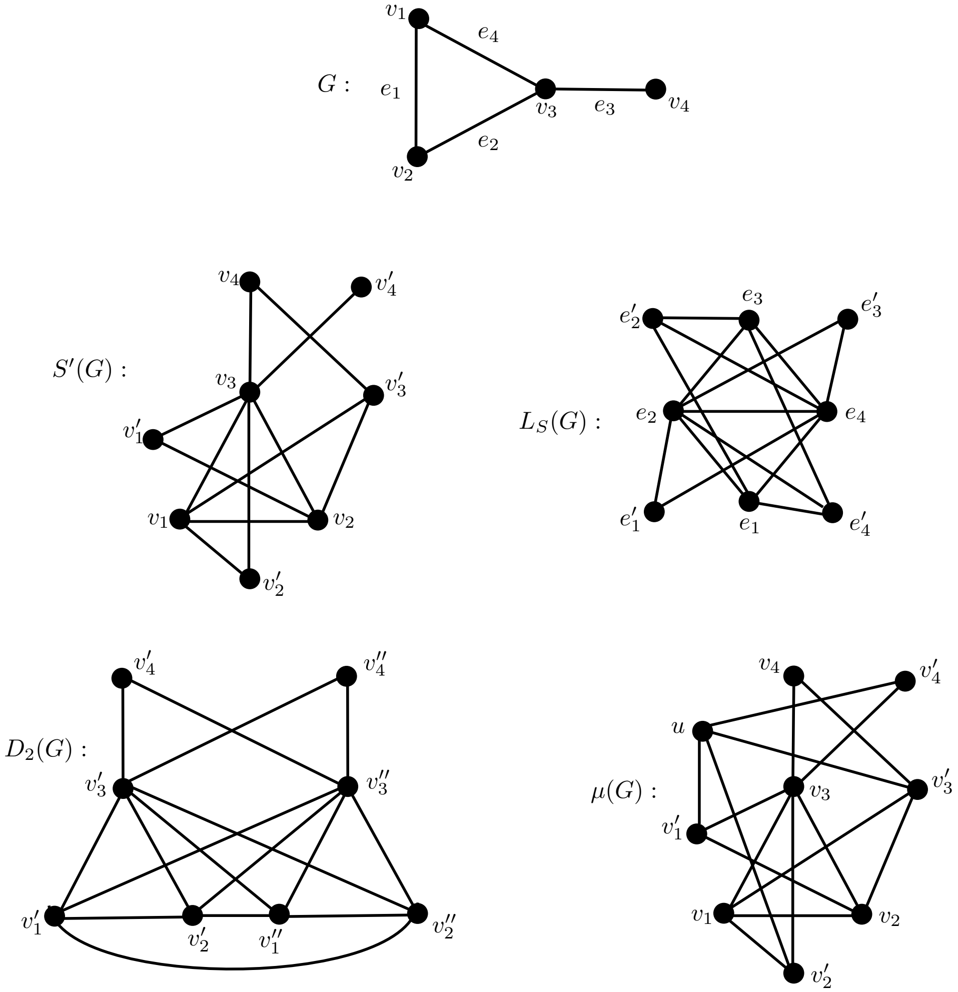

FIGURE 1. The graph G with its vertex splitting graph $S'(G)$, line splitting graph $L_s(G)$, shadow graph $D_2(G)$ and Mycielskian $\mu(G)$.

Theorem 2.6. *If* G *is a graph of order* n *and size* m *with the* M*-polynomial* $M(G;x,y)=\sum\limits_{i\leq j} m_{ij}(G)x^iy^j$, *then*

$$M(\mu(G);x,y)=\sum_{i\leq j} m_{ij}(G)x^{2i}y^{2j}+\sum_{a'\leq b'} m_{a'b'}(G)x^{a'}y^{b'},$$

where $a'=min\{a,b\}, b'=max\{a,b\}$, *and for* $i'=min\{i,j\}, j'=max\{i,j\}$

$$m_{a'b'}(G)=\begin{cases} m_{i'j'}(G) & if\ a=i+1, b=2j \quad and\ \ i\neq j,\\ 2m_{i'j'}(G) & if\ a=i+1, b=2j \quad and\ \ i=j,\\ |\{v:d_v=i\}| & if\ a=i+1, b=n \quad for\ \ i=1,2,...,n-1.\end{cases}$$

Proof. By definition of mycielskian of a graph, we have the degree of the original vertices of G in $\mu(G)$ is twice the degree of that vertex in G, the degree $d_{\mu(G)}(v_i')=d_G(v_i)+1$ of the duplicates v_i' of $v_i\in V(G)$ and the degree of the vertex $u\in\mu(G)$

is n. Therefore, we have the following:

$$m_{2i2j}(\mu(G)) = m_{ij}(G)$$

and

$$m_{a'b'}(G) = \begin{cases} m_{i'j'}(G) & if\ a = i+1, b = 2j \quad and\ \ i \neq j, \\ 2m_{i'j'}(G) & if\ a = i+1, b = 2j \quad and\ \ i = j, \\ |\{v : d_v = i\}| & if\ a = i+1, b = n \quad for\ \ i = 1, 2, ..., n-1. \end{cases}$$

Thus, we get the desired result by substituting these values in Eq. (1.1). □

Corollary 2.7. *If M-polynomial of Mycielskian of a graph G is*

$$M(\mu(G); x, y) = \sum_{i \leq j} m_{ij}(G) x^{2i} y^{2j} + \sum_{a' \leq b'} m_{a'b'}(G) x^{a'} y^{b'},$$

then

$$\begin{aligned} M_1(\mu(G)) &= 2\sum_{i \leq j}(i+j)m_{ij}(G) + \sum_{a' \leq b'}(a'+b')m_{a'b'}(G), \\ M_2(\mu(G)) &= 4\sum_{i \leq j} ij m_{ij}(G) + \sum_{a' \leq b'} a'b' m_{a'b'}(G), \\ {}^{m}M_2(\mu(G)) &= \frac{1}{4}\sum_{i \leq j}\frac{m_{ij}(G)}{ij} + \sum_{a' \leq b'}\frac{m_{a'b'}(G)}{a'b'}, \\ S_D(\mu(G)) &= \sum_{i \leq j}\frac{(i^2+j^2)m_{ij}(G)}{ij} + \sum_{a' \leq b'}\frac{(a'^2+b'^2)m_{a'b'}(G)}{a'b'}, \\ H(\mu(G)) &= \sum_{i \leq j}\frac{ij m_{ij}(G)}{(i+j)} + 2\sum_{a' \leq b'}\frac{a'b' m_{a'b'}(G)}{(a'+b')}, \\ I_n(\mu(G)) &= \sum_{i \leq j} ij(i+j)m_{ij}(G) + \sum_{a' \leq b'} a'b'(a'+b')m_{a'b'}(G). \end{aligned}$$

Proof. We get the desired results by applying the appropriate operators to M-polynomial of $\mu(G)$. □

Definition 6. [8] *Let P_3 be the 3-vertex tree rooted at one its terminal vertices. See Fig. 2. For $k = 2, 3, ...$ construct the rooted tree B_k by identifying the roots of k copies of P_3. The vertex obtained by identifying the roots of P_3-trees is the root of B_k. The illustrative structure of the rooted tree B_k is depicted in Fig. 2*

Definition 7. [8] *Let d be an integer and $\beta_1, \beta_2, ..., \beta_d$ be rooted trees as specified in Definition 6, i.e., $\beta_1, \beta_2, ..., \beta_d \in \{B_2, B_3, ...\}$. A Kragujevac tree T_k is a tree possessing a vertex of degree d, adjacent to the roots of $\beta_1, \beta_2, ..., \beta_d$. This vertex is said to be the central vertex of T_k. The subgraphs $\beta_1, \beta_2, ..., \beta_d$ are the branches of T_k. Note that, some (or all) branches of T_k may be mutually isomorphic.*

Theorem 2.8. *If T_k is a Kragujevac tree with $\beta_1, \beta_2, ..., \beta_d \in \{B_2, B_3, ...\}$ branches, then*

$$M(T_k; x, y) = \sum_{i \geq 2} i k_i x y^2 + \sum_{i \geq 2} i k_i x^2 y^{i+1} + \sum_{i \geq 2} k_i x^d y^{i+1},$$

where $k_i = |\{\beta_i : \beta_i$ is a branch of T_k such that $\beta_i = B_i\}|$ for $i \geq 2$.

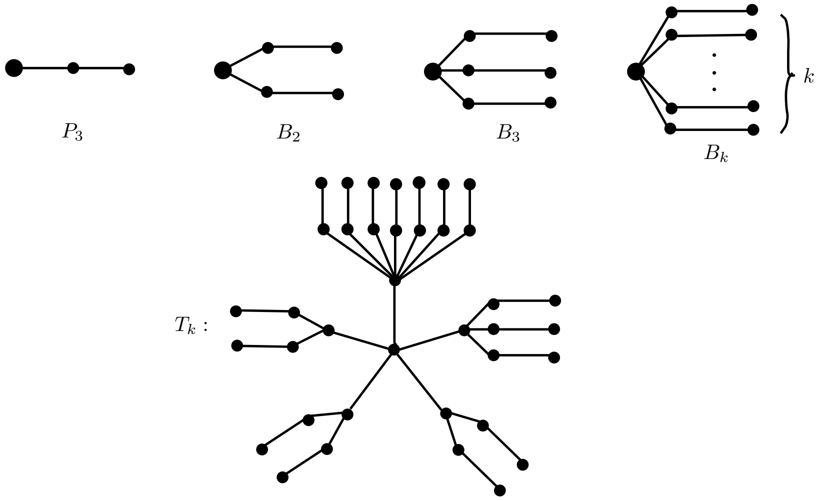

Figure 2. The rooted trees B_k's and the Kragujevac tree T_k.

Proof. By definition of Kragujevac tree T_k, we have $\sum_{i\geq 2} ik_i$ vertices of degree 1, $\sum_{i\geq 2} ik_i$ vertices of degree 2 and k_i vertices of degree $i+1$. Therefore, the edge partition of T_k is given as follows:

$$\begin{aligned}
|E_{\{1,2\}}| &= |uv \in E(T_k) : d_u = 1 \ \ and \ \ d_v = 2| = \sum_{i\geq 2} ik_i, \\
|E_{\{2,i+1\}}| &= |uv \in E(T_k) : d_u = 2 \ \ and \ \ d_v = i+1| = ik_i, \\
|E_{\{d,i+1\}}| &= |uv \in E(T_k) : d_u = d \ \ and \ \ d_v = i+1| = k_i.
\end{aligned}$$

Thus, the $M-polynomial$ of T_k is

$$M(T_k;x,y) = \sum_{i\leq j} m_{ij}(T_k)x^i y^j = \sum_{i\geq 2} ik_i xy^2 + \sum_{i\geq 2} ik_i x^2 y^{i+1} + \sum_{i\geq 2} k_i x^d y^{i+1}.$$

□

Corollary 2.9. *If M-polynomial of Kragujevac tree T_k is*

$$M(T_k;x,y) = \sum_{i\geq 2} ik_i xy^2 + \sum_{i\geq 2} ik_i x^2 y^{i+1} + \sum_{i\geq 2} k_i x^d y^{i+1},$$

then

$$\begin{aligned}
M_1(T_k) &= \sum_{i\geq 2}(i^2+7i+d+1)k_i,\\
M_2(T_k) &= \sum_{i\geq 2}(2i^2+(4+d)i+d)k_i,\\
{}^mM_2(T_k) &= \sum_{i\geq 2}\frac{(i^2+5i+2d)}{2(i+1)}k_i,\\
S_D(T_k) &= \sum_{i\geq 2}\frac{(7i^2+13i+2d+2)}{2(i+1)}k_i,\\
H(T_k) &= \sum_{i\geq 2}\frac{(2i^3+2(d+7)i^2+6(2d+3)i+18)}{3(i+3)(d+i+1)}k_i,\\
I_n(T_k) &= \sum_{i\geq 2}\frac{(8i^3+(11d+20)i^2+12(2d+1)i+9d)}{3(i+3)(d+i+1)}k_i.
\end{aligned}$$

Proof. We get the desired results by applying the appropriate operators on M-polynomial of T_k. □

The definitions of the special graphs used in this paper can be found in [9]. In this section, we obtain $M-$ polynomials of some special graphs. We also derive some topological indices (mentioned in section 1) of these graphs from the respective $M-$ polynomials.

Definition 8. *The book graph $B_m = S_m \times P_2$ is a graph with $2(m+1)$ vertices and $(3m+1)$ edges, where S_m is a star of order $(m+1)$ and P_2 is a path of length one.*

Theorem 2.10. *If B_m is a book graph of order $2(m+1)$ and size $(3m+1)$, then*

$$M(B_m;x,y) = mx^2y^2 + 2mx^2y^{m+1} + x^{m+1}y^{m+1}.$$

Proof. The book graph B_m has $2(m+1)$ vertices and $(3m+1)$ edges. The edge set of B_m can be partitioned as,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(B_m) : d_u = 2 \;\; and \;\; d_v = 2| = m,\\
|E_{\{2,m+1\}}| &= |uv \in E(B_m) : d_u = 2 \;\; and \;\; d_v = m+1| = 2m,\\
|E_{\{m+1,m+1\}}| &= |uv \in E(B_m) : d_u = m+1 \;\; and \;\; d_v = m+1|\\
&= |E(B_m) - |E_{\{2,2\}}| - |E_{\{2,m+1\}}| = 1.
\end{aligned}$$

Thus, the $M-polynomial$ of B_m is
$$M(B_m;x,y) = \sum_{i\leq j} m_{ij}(B_m)x^iy^j = mx^2y^2 + 2mx^2y^{m+1} + x^{m+1}y^{m+1}.$$
□

Corollary 2.11. *If M-polynomial of the book graph B_m is $M(B_m;x,y) = mx^2y^2 + 2mx^2y^{m+1} + x^{m+1}y^{m+1}$, then*

$$\begin{aligned}
M_1(B_m) &= 2(m^2+6m+1),\\
M_2(B_m) &= 5m^2+10m+1,\\
{}^mM_2(B_m) &= \frac{m^3+6m^2+5m+4}{4(m^2+2m+1)},\\
S_D(B_m) &= \frac{m^3+4m^2+9m+2}{m+1},\\
H(B_m) &= \frac{m^3+12m^2+13m+6}{2(m^2+4m+3)},\\
I_n(B_m) &= \frac{11m^2+18m+3}{2(m+3)}.
\end{aligned}$$

Proof. We have, the M-polynomial of the book graph B_m as

$$M(B_m;x,y) = mx^2y^2 + 2mx^2y^{m+1} + x^{m+1}y^{m+1}.$$

Therefore,

$$\begin{aligned}
D_x &= x\frac{\partial f(x,y)}{\partial x} = 2mx^2y^2 + 4mx^2y^{m+1} + (m+1)x^{m+1}y^{m+1},\\
D_y &= y\frac{\partial f(x,y)}{\partial y} = 2mx^2y^2 + 2m(m+1)x^2y^{m+1} + (m+1)x^{m+1}y^{m+1},\\
S_x &= \int_0^x \frac{f(t,y)}{t}dt = \frac{m}{2}x^2y^2 + mx^2y^{m+1} + \frac{1}{(m+1)}x^{m+1}y^{m+1},\\
S_y &= \int_0^y \frac{f(x,t)}{t}dt = \frac{m}{2}x^2y^2 + \frac{2m}{(m+1)}x^2y^{m+1} + \frac{1}{(m+1)}x^{m+1}y^{m+1},\\
J(f(x,y)) &= f(x,x) = mx^4 + 2mx^{m+3} + x^{2(m+1)}.
\end{aligned}$$

Thus, we get

$$\begin{aligned}
M_1(B_m) &= (D_x+D_y)(M(B_m;x,y))|_{x=y=1} = 2(m^2+6m+1),\\
M_2(B_m) &= (D_xD_y)(M(B_m;x,y))|_{x=y=1} = 5m^2+10m+1,\\
{}^mM_2(B_m) &= (S_xS_y)(M(B_m;x,y))|_{x=y=1} = \frac{m^3+6m^2+5m+4}{4(m^2+2m+1)},\\
S_D(B_m) &= (D_xS_y+D_yS_x)(M(B_m;x,y))|_{x=y=1} = \frac{m^3+4m^2+9m+2}{m+1},\\
H(B_m) &= 2S_xJ(M(B_m;x,y))|_{x=1} = \frac{m^3+12m^2+13m+6}{2(m^2+4m+3)},\\
I_n(B_m) &= S_xJD_xD_y(M(B_m;x,y))|_{x=1} = \frac{11m^2+18m+3}{2(m+3)}.
\end{aligned}$$

□

Definition 9. *The Ladder $L_n = P_n \times P_2$ is a graph of order $2n$ and size $(3n-2)$, where P_n and P_2 are two paths of length $(n-1)$ and 1, respectively.*

Theorem 2.12. *If L_n is a ladder, then*

$$M(L_n;x,y) = 2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3.$$

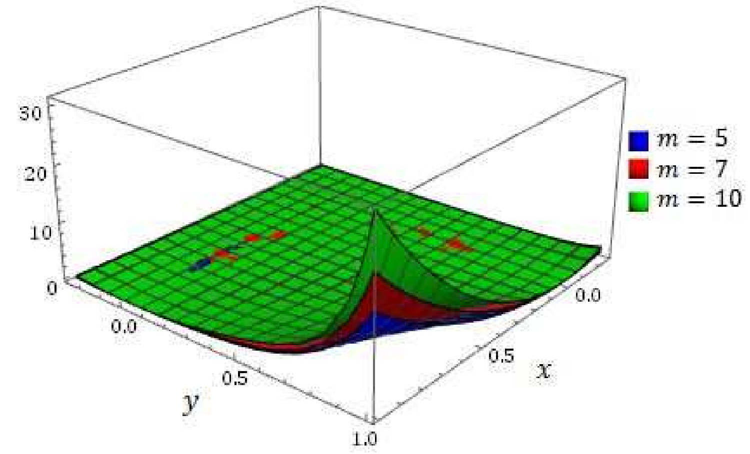

FIGURE 3. Plot of M-polynomial of the book graph B_{10}

Proof. The ladder L_n has $2n$ vertices and $(3n-2)$ edges. The edge set of L_n can be partitioned as,

$$\begin{aligned}|E_{\{2,2\}}| &= |uv \in E(L_n) : d_u = 2 \;\; and \;\; d_v = 2| = 2,\\ |E_{\{2,3\}}| &= |uv \in E(L_n) : d_u = 2 \;\; and \;\; d_v = 3| = 4,\\ |E_{\{3,3\}}| &= |uv \in E(L_n) : d_u = 3 \;\; and \;\; d_v = 3|\\ &= |E(L_n) - |E_{\{2,2\}}| - |E_{\{2,3\}}| = 3n - 8.\end{aligned}$$

Thus, the $M-polynomial$ of L_n is

$$M(L_n; x, y) = \sum_{i \leq j} m_{ij}(L_n)x^i y^j = 2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3. \qquad \square$$

Corollary 2.13. *If the M-polynomial of the ladder L_n is $M(L_n; x, y) = 2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3$, then*

$$\begin{aligned}M_1(L_n) &= 2(9n-10),\\ M_2(L_n) &= 27n-40,\\ {}^mM_2(L_n) &= \frac{6n+5}{18},\\ S_D(L_n) &= \frac{2(9n-5)}{3},\\ H(L_n) &= \frac{15n-1}{15},\\ I_n(L_n) &= \frac{45n-52}{10}.\end{aligned}$$

Proof. We have, the M-polynomial of the ladder L_n as

$$M(L_n; x, y) = 2x^2y^2 + 4x^2y^3 + (3n-8)x^3y^3.$$

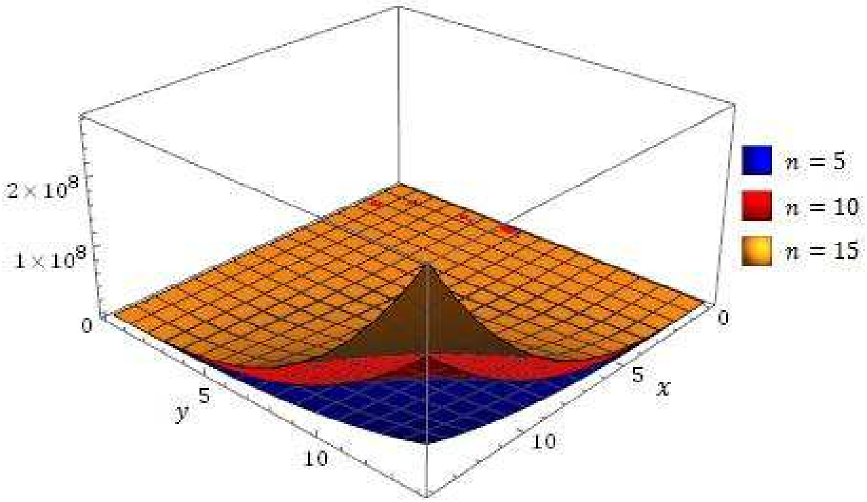

Figure 4. Plot of M-polynomial of the ladder L_{10}

Therefore,

$$\begin{aligned}
D_x &= x\frac{\partial f(x,y)}{\partial x} = 4x^2y^2 + 8x^2y^3 + 3(3n-8)x^3y^3, \\
D_y &= y\frac{\partial f(x,y)}{\partial y} = 4x^2y^2 + 12x^2y^3 + 3(3n-8)x^3y^3, \\
S_x &= \int_0^x \frac{f(t,y)}{t}dt = x^2y^2 + 2x^2y^3 + \frac{(3n-8)}{3}x^3y^3, \\
S_y &= \int_0^y \frac{f(x,t)}{t}dt = x^2y^2 + \frac{4}{3}x^2y^3 + \frac{(3n-8)}{3}x^3y^3, \\
J(f(x,y)) &= f(x,x) = 2x^4 + 4x^5 + (3n-8)x^6.
\end{aligned}$$

Thus, we get

$$\begin{aligned}
M_1(L_n) &= (D_x + D_y)(M(L_n;x,y))|_{x=y=1} = 2(9n-10), \\
M_2(L_n) &= (D_xD_y)(M(L_n;x,y))|_{x=y=1} = 27n-40, \\
{}^mM_2(L_n) &= (S_xS_y)(M(L_n;x,y))|_{x=y=1} = \frac{6n+5}{18}, \\
S_D(L_n) &= (D_xS_y + D_yS_x)(M(L_n;x,y))|_{x=y=1} = \frac{2(9n-5)}{3}, \\
H(L_n) &= 2S_xJ(M(L_n;x,y))|_{x=1} = \frac{15n-1}{15}, \\
I_n(L_n) &= S_xJD_xD_y(M(L_n;x,y))|_{x=1} = \frac{45n-52}{10}.
\end{aligned}$$

□

The surfaces in Figures 3 and 4 are plotted by using Mathematica. These surfaces are obtained by M-polynomial of the respective graph which shows different behaviours for different parameters m, n, x and y.

Definition 10. *A planar grid $P_m \times P_n$, is a graph obtained by the product of two paths P_m and P_n of lengths $(m-1)$ and $(n-1)$, respectively.*

Theorem 2.14. *If $P_m \times P_n$ is a planar grid, then*
$M(P_m \times P_n; x, y) = 8x^2y^3 + 2(m+n-6)x^3y^3 + 2(m+n-4)x^3y^4 + (2mn-5m-5n+12)x^4y^4.$

Proof. The planar grid $P_m \times P_n$ has mn vertices and $(2mn-m-n)$ edges. The edge set of $P_m \times P_n$ can be partitioned as,

$$\begin{aligned}
|E_{\{2,3\}}| &= |uv \in E(P_m \times P_n) : d_u = 2 \ \ and \ \ d_v = 3| = 8,\\
|E_{\{3,3\}}| &= |uv \in E(P_m \times P_n) : d_u = 3 \ \ and \ \ d_v = 3| = 2(m+n-6),\\
|E_{\{3,4\}}| &= |uv \in E(P_m \times P_n) : d_u = 3 \ \ and \ \ d_v = 4| = 2(m+n-4),\\
|E_{\{4,4\}}| &= |uv \in E(P_m \times P_n) : d_u = 4 \ \ and \ \ d_v = 4|\\
&= |E(P_m \times P_n) - |E_{\{2,3\}}| - |E_{\{3,3\}}| - |E_{\{3,4\}}| = 2mn - 5m - 5n + 12.
\end{aligned}$$

Thus, the $M-polynomial$ of $P_m \times P_n$ is

$$\begin{aligned}
M(P_m \times P_n; x, y) &= \sum_{i \le j} m_{ij}(P_m \times P_n)x^iy^j\\
&= 8x^2y^3 + 2(m+n-6)x^3y^3 + 2(m+n-4)x^3y^4 + (2mn-5m-5n+12)x^4y^4.
\end{aligned}$$

□

Definition 11. *The prism $\Pi_n = C_n \times P_2$ is a 3-regular graph of order $2n$ and size $3n$, where C_n is cycle of order n and P_2 is a path of length one.*

Theorem 2.15. *If Π_n is a prism, then*

$$M(\Pi_n; x, y) = 3nx^3y^3.$$

Proof. Let prism Π_n be a 3-regular graph having $2n$ vertices and $3n$ edges. The edge partition of Π_n is given by,

$$|E_{\{3,3\}}| = |uv \in E(\Pi_n) : d_u = 3 \ \ and \ \ d_v = 3| = 3n.$$

Thus, the $M-polynomial$ of the prism Π_n is

$$M(\Pi_n; x, y) = \sum_{i \le j} m_{ij}(\Pi_n)x^iy^j = 3nx^3y^3.$$

□

Definition 12. *The book graph with triangular pages $B_m^t = P_2 + mK_1$ is a graph with $(n+2)$ vertices and $(2n+1)$ edges, where P_2 is a path of length one and mK_1 are the m isolated vertices.*

Theorem 2.16. *If B_m^t is a book graph with triangular pages having $(n+2)$ vertices and $(2n+1)$ edges, then*

$$M(B_m^t; x, y) = 2mx^2y^{m+1} + x^{m+1}y^{m+1}.$$

Proof. Let B_m^t is a book graph with triangular pages having $(n+2)$ vertices and $(2n+1)$ edges. The edge partition of B_m^t is given by,

$$\begin{aligned}
|E_{\{2,m+1\}}| &= |uv \in E(B_m^t) : d_u = 2 \ \ and \ \ d_v = m+1| = 2m,\\
|E_{\{m+1,m+1\}}| &= |uv \in E(B_m^t) : d_u = m+1 \ \ and \ \ d_v = m+1|\\
&= |E(B_m^t) - |E_{\{2,m+1\}}| = 1.
\end{aligned}$$

Thus, $M(B_m^t; x, y) = \sum_{i \le j} m_{ij}(B_m^t)x^iy^j = 2mx^2y^{m+1} + x^{m+1}y^{m+1}.$ □

Definition 13. *The corona $P_n \circ K_1$ of a path P_n of length $(n-1)$ with an isolated vertex K_1 is called a comb graph and the corona $P_n \circ 2K_1$ of a path P_n of length $(n-1)$ with two isolated vertices $2K_1$ is called a double comb graph.*

Theorem 2.17. *If $P_n \circ K_1$ is a comb graph, then*

$$M(P_n \circ K_1; x, y) = 2xy^2 + (n-2)xy^3 + 2x^2y^3 + (n-3)x^3y^3.$$

Proof. The comb graph $P_n \circ K_1$ has $2n$ vertices and $(2n-1)$ edges. The edge set of $P_n \circ K_1$ can be partitioned as,

$$\begin{aligned}
|E_{\{1,2\}}| &= |uv \in E(P_n \circ K_1) : d_u = 1 \;\; and \;\; d_v = 2| = 2,\\
|E_{\{1,3\}}| &= |uv \in E(P_n \circ K_1) : d_u = 1 \;\; and \;\; d_v = 3| = (n-2),\\
|E_{\{2,3\}}| &= |uv \in E(P_n \circ K_1) : d_u = 2 \;\; and \;\; d_v = 3| = 2,\\
|E_{\{3,3\}}| &= |uv \in E(P_n \circ K_1) : d_u = 3 \;\; and \;\; d_v = 3|\\
&= |E(P_n \circ K_1) - |E_{\{1,2\}}| - |E_{\{1,3\}}| - |E_{\{2,3\}}| = n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of $P_n \circ K_1$ is

$$\begin{aligned}
M(P_n \circ K_1; x, y) &= \sum_{i \leq j} m_{ij}(P_n \circ K_1)x^iy^j\\
&= 2xy^2 + (n-2)xy^3 + 2x^2y^3 + (n-3)x^3y^3.
\end{aligned}$$

□

Theorem 2.18. *If $P_n \circ 2K_1$ is a double comb graph, then*

$$M(P_n \circ 2K_1; x, y) = 4xy^3 + 2(n-2)xy^4 + 2x^3y^4 + (n-3)x^4y^4.$$

Proof. The double comb graph $P_n \circ 2K_1$ has $3n$ vertices and $(3n-1)$ edges. The edge set of $P_n \circ 2K_1$ can be partitioned as,

$$\begin{aligned}
|E_{\{1,3\}}| &= |uv \in E(P_n \circ 2K_1) : d_u = 1 \;\; and \;\; d_v = 3| = 4,\\
|E_{\{1,4\}}| &= |uv \in E(P_n \circ 2K_1) : d_u = 1 \;\; and \;\; d_v = 4| = 2(n-2),\\
|E_{\{3,4\}}| &= |uv \in E(P_n \circ 2K_1) : d_u = 3 \;\; and \;\; d_v = 4| = 2,\\
|E_{\{4,4\}}| &= |uv \in E(P_n \circ 2K_1) : d_u = 4 \;\; and \;\; d_v = 4|\\
&= |E(P_n \circ 2K_1) - |E_{\{1,3\}}| - |E_{\{1,4\}}| - |E_{\{3,4\}}| = n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of $P_n \circ 2K_1$ is

$$\begin{aligned}
M(P_n \circ 2K_1; x, y) &= \sum_{i \leq j} m_{ij}(P_n \circ 2K_1)x^iy^j\\
&= 4xy^3 + 2(n-2)xy^4 + 2x^3y^4 + (n-3)x^4y^4.
\end{aligned}$$

□

Definition 14. *A jelly fish $J(m, n)$ is a graph obtained from a cycle $C_4 : uxvyu$ by joining x and y with an edge and appending m pendant edges to u and n pendant edges to v.*

Theorem 2.19. *If $J(m, n)$ is a jelly fish graph, then*

$$M(J(m, n); x, y) = mxy^{m+2} + nxy^{n+2} + 2x^3y^{m+2} + 2x^3y^{n+2} + x^3y^3.$$

Proof. The jelly fish graph $J(m,n)$ has $(4+m+n)$ vertices and $(5+m+n)$ edges. The edge set of $J(m,n)$ can be partitioned as,

$$\begin{aligned}
|E_{\{1,m+2\}}| &= |uv \in E(J(m,n)) : d_u = 1 \;\; and \;\; d_v = m+2| = m,\\
|E_{\{1,n+2\}}| &= |uv \in E(J(m,n)) : d_u = 1 \;\; and \;\; d_v = n+2| = n,\\
|E_{\{3,m+2\}}| &= |uv \in E(J(m,n)) : d_u = 3 \;\; and \;\; d_v = m+2| = 2,\\
|E_{\{3,n+2\}}| &= |uv \in E(J(m,n)) : d_u = 3 \;\; and \;\; d_v = n+2| = 2,\\
|E_{\{3,3\}}| &= |uv \in E(J(m,n)) : d_u = 3 \;\; and \;\; d_v = 3|\\
&= |E(J(m,n)) - |E_{\{1,m+2\}}| - |E_{\{1,n+2\}}| - |E_{\{3,m+2\}}| - |E_{\{3,n+2\}}| = 1.
\end{aligned}$$

Thus, the $M-polynomial$ of $J(m,n)$ is

$$\begin{aligned}
M(J(m,n);x,y) &= \sum_{i\leq j} m_{ij}(J(m,n))x^i y^j\\
&= mxy^{m+2} + nxy^{n+2} + 2x^3y^{m+2} + 2x^3y^{n+2} + x^3y^3.
\end{aligned}$$

□

Definition 15. *A butterfly graph $By_{m,n}$ is obtained from two even cycles of the same order n for $n \geq 3$, sharing a common vertex with m pendant edges attached at the common vertex.*

Theorem 2.20. *If $By_{m,n}$ is a butterfly graph, then*

$$M(By_{m,n};x,y) = mxy^{m+4} + 4x^2y^{m+4} + (2n-4)x^2y^2.$$

Proof. The butterfly graph $By_{m,n}$ has $(2n+m-1)$ vertices and $(2n+m)$ edges. The edge set of $By_{m,n}$ can be partitioned as,

$$\begin{aligned}
|E_{\{1,m+4\}}| &= |uv \in E(By_{m,n}) : d_u = 1 \;\; and \;\; d_v = m+4| = m,\\
|E_{\{2,m+4\}}| &= |uv \in E(By_{m,n}) : d_u = 2 \;\; and \;\; d_v = m+4| = 4,\\
|E_{\{2,2\}}| &= |uv \in E(By_{m,n}) : d_u = 2 \;\; and \;\; d_v = 2|\\
&= |E(By_{m,n}) - |E_{\{1,m+4\}}| - |E_{\{2,m+4\}}| = 2n-4.
\end{aligned}$$

Thus, the $M-polynomial$ of $By_{m,n}$ is

$$\begin{aligned}
M(By_{m,n};x,y) &= \sum_{i\leq j} m_{ij}(By_{m,n})x^i y^j\\
&= mxy^{m+4} + 4x^2y^{m+4} + (2n-4)x^2y^2.
\end{aligned}$$

□

Definition 16. *The triangular snake [17] T_n is a graph obtained from the path P_n of length $(n-1)$, by replacing each edge of the path by a triangle C_3.*

Theorem 2.21. *If T_n is a triangular snake, then*

$$M(T_n;x,y) = 2x^2y^2 + 2(n-1)x^2y^4 + (n-3)x^4y^4.$$

Proof. Let triangular snake T_n be a graph having $(2n-1)$ vertices and $3(n-1)$ edges. The edge partition of T_n is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(T_n) : d_u = 2 \;\; and \;\; d_v = 2| = 2,\\
|E_{\{2,4\}}| &= |uv \in E(T_n) : d_u = 2 \;\; and \;\; d_v = 4| = 2(n-1),\\
|E_{\{4,4\}}| &= |uv \in E(T_n) : d_u = 4 \;\; and \;\; d_v = 4|\\
&= |E(T_n)| - |E_{\{2,2\}}| - |E_{\{2,4\}}| = n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of T_n is

$$M(T_n;x,y)=\sum_{i\leq j} m_{ij}(T_n)x^iy^j=2x^2y^2+2(n-1)x^2y^4+(n-3)x^4y^4.$$

□

Definition 17. *The double triangular snake* DT_n *is a graph consisting of two triangular snakes that have a common path. i.e., a double triangular snake is obtained from the path* $P_n: u_1u_2...u_n$ *by joining* u_i *and* u_{i+1} *to a new vertex* $v_i,(1\leq i\leq n-1)$ *and to a new vertex* $w_i,(1\leq i\leq n-1)$.

Theorem 2.22. *If* DT_n *is a double triangular snake, then*

$$M(DT_n;x,y)=4x^2y^3+4(n-2)x^2y^6+2x^3y^6+(n-3)x^6y^6.$$

Proof. Let double triangular snake DT_n be a graph having $(3n-2)$ vertices and $5(n-1)$ edges. The edge partition of DT_n is given by,

$$\begin{aligned}
|E_{\{2,3\}}| &= |uv\in E(DT_n): d_u=2 \ \ and \ \ d_v=3|=4,\\
|E_{\{2,6\}}| &= |uv\in E(DT_n): d_u=2 \ \ and \ \ d_v=6|=4(n-2),\\
|E_{\{3,6\}}| &= |uv\in E(DT_n): d_u=3 \ \ and \ \ d_v=6|=2,\\
|E_{\{6,6\}}| &= |uv\in E(DT_n): d_u=6 \ \ and \ \ d_v=6|\\
&= |E(DT_n)|-|E_{\{2,3\}}|-|E_{\{2,6\}}|-|E_{\{3,6\}}|=n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of DT_n is

$$M(DT_n;x,y)=\sum_{i\leq j} m_{ij}(DT_n)x^iy^j=4x^2y^3+4(n-2)x^2y^6+2x^3y^6+(n-3)x^6y^6.$$

□

Definition 18. *An irregular triangular snake* IT_n *is a graph obtained from the path* $P_n: u_1u_2...u_n$ *with vertex set* $V(IT_n)=V(P_n)\cup\{v_i: 1\leq i\leq n-2\}$ *and the edge set* $E(IT_n)=E(P_n)\cup\{u_iv_i, v_iu_{i+2}: 1\leq i\leq n-2\}$.

Theorem 2.23. *If* IT_n *is an irregular triangular snake, then*

$$M(IT_n;x,y)=2x^2y^2+4x^2y^3+2x^3y^4+2(n-4)x^2y^4+(n-5)x^4y^4.$$

Proof. Let an irregular triangular snake IT_n be a graph having $2(n-1)$ vertices and $(3n-5)$ edges. The edge partition of IT_n is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv\in E(IT_n): d_u=2 \ \ and \ \ d_v=2|=2,\\
|E_{\{2,3\}}| &= |uv\in E(IT_n): d_u=2 \ \ and \ \ d_v=3|=4,\\
|E_{\{2,4\}}| &= |uv\in E(IT_n): d_u=2 \ \ and \ \ d_v=4|=2(n-4),\\
|E_{\{3,4\}}| &= |uv\in E(IT_n): d_u=3 \ \ and \ \ d_v=4|=2,\\
|E_{\{4,4\}}| &= |uv\in E(IT_n): d_u=4 \ \ and \ \ d_v=4|\\
&= |E(IT_n)|-|E_{\{2,2\}}|-|E_{\{2,3\}}|-|E_{\{2,4\}}|-|E_{\{3,4\}}|=n-5.
\end{aligned}$$

Thus, the $M-polynomial$ of IT_n is

$$M(IT_n;x,y)=\sum_{i\leq j} m_{ij}(IT_n)x^iy^j=2x^2y^2+4x^2y^3+2x^3y^4+2(n-4)x^2y^4+(n-5)x^4y^4.$$

□

Definition 19. *The alternate triangular snake $A(T_n)$ is obtained from a path $v_1v_2...v_n$ by joining v_i and v_{i+1} (alternatively) to new vertex v_i, that is, every alternate edge of a path is replaced by C_3.*

Theorem 2.24. *If $A(T_n)$ is an alternate triangular snake, then*

$$M(A(T_n);x,y) = \begin{cases} 2x^2y^2 + nx^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is even}, \\ xy^3 + x^2y^2 + (n-1)x^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is odd}. \end{cases}$$

Proof. Let an alternate triangular snake $A(T_n)$ be a graph having $(n+\lfloor\frac{n}{2}\rfloor)$ vertices and $(n-1+\lfloor\frac{n}{2}\rfloor)$ edges. The edge partition of $A(T_n)$ is given as follows:
If n is even, then there will be no pendant edge in $A(T_n)$. Therefore, we have

$$\begin{aligned} |E_{\{2,2\}}| &= |uv \in E(A(T_n)) : d_u = 2 \;\; and \;\; d_v = 2| = 2, \\ |E_{\{2,3\}}| &= |uv \in E(A(T_n)) : d_u = 2 \;\; and \;\; d_v = 3| = n, \\ |E_{\{3,3\}}| &= |uv \in E(A(T_n)) : d_u = 3 \;\; and \;\; d_v = 3| \\ &= |E(A(T_n))| - |E_{\{2,2\}}| - |E_{\{2,3\}}| = n-3. \end{aligned}$$

If n is odd, then there will be a pendant edge in $A(T_n)$. Therefore, we have

$$\begin{aligned} |E_{\{1,3\}}| &= |uv \in E(A(T_n)) : d_u = 1 \;\; and \;\; d_v = 3| = 1, \\ |E_{\{2,2\}}| &= |uv \in E(A(T_n)) : d_u = 2 \;\; and \;\; d_v = 2| = 1, \\ |E_{\{2,3\}}| &= |uv \in E(A(T_n)) : d_u = 2 \;\; and \;\; d_v = 3| = n-1, \\ |E_{\{3,3\}}| &= |uv \in E(A(T_n)) : d_u = 3 \;\; and \;\; d_v = 3| \\ &= |E(A(T_n))| - |E_{\{1,3\}}| - |E_{\{2,2\}}| - |E_{\{2,3\}}| = n-3. \end{aligned}$$

Thus, the $M-polynomial$ of $A(T_n)$ is

$$M(A(T_n);x,y) = \sum_{i\leq j} m_{ij}(A(T_n))x^iy^j = \begin{cases} 2x^2y^2 + nx^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is even}, \\ xy^3 + x^2y^2 + (n-1)x^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is odd}. \end{cases}$$

□

Definition 20. *A double alternate triangular snake $DA(T_n)$ consists of two alternate triangular snakes that have a common path.*

Theorem 2.25. *Let $DA(T_n)$ be a double alternate triangular snake. Then*

$$M(DA(T_n);x,y) = \begin{cases} 4x^2y^3 + (4\left\lfloor\frac{n}{2}\right\rfloor - 4)x^2y^4 + 2x^3y^4 + (n-3)x^4y^4 & \text{if } n \text{ is even}, \\ xy^4 + 2x^2y^3 + (4\left\lfloor\frac{n}{2}\right\rfloor - 2)x^2y^4 + x^3y^4 + (n-3)x^4y^4 & \text{if } n \text{ is odd}. \end{cases}$$

Proof. Let a double alternate triangular snake $DA(T_n)$ be a graph having $(n+2\lfloor\frac{n}{2}\rfloor)$ vertices and $(n-1+4\lfloor\frac{n}{2}\rfloor)$ edges. The edge partition of $DA(T_n)$ is given as follows:
If n is even, then there will be no pendant edge in $DA(T_n)$. Therefore, we have

$$\begin{aligned} |E_{\{2,3\}}| &= |uv \in E(DA(T_n)) : d_u = 2 \;\; and \;\; d_v = 3| = 4, \\ |E_{\{2,4\}}| &= |uv \in E(DA(T_n)) : d_u = 2 \;\; and \;\; d_v = 4| = 4\left\lfloor\frac{n}{2}\right\rfloor - 4, \\ |E_{\{3,4\}}| &= |uv \in E(DA(T_n)) : d_u = 3 \;\; and \;\; d_v = 4| = 2, \\ |E_{\{4,4\}}| &= |uv \in E(DA(T_n)) : d_u = 4 \;\; and \;\; d_v = 4| \\ &= |E(DA(T_n))| - |E_{\{2,3\}}| - |E_{\{2,4\}}| - |E_{\{3,4\}}| = n-3. \end{aligned}$$

If n is odd, then there will be a pendant edge in $DA(T_n)$. Therefore, we have

$$\begin{aligned}
|E_{\{1,4\}}| &= |uv \in E(DA(T_n)) : d_u = 1 \ \textit{and} \ d_v = 4| = 1,\\
|E_{\{2,3\}}| &= |uv \in E(DA(T_n)) : d_u = 2 \ \textit{and} \ d_v = 3| = 2,\\
|E_{\{2,4\}}| &= |uv \in E(DA(T_n)) : d_u = 2 \ \textit{and} \ d_v = 4| = 4\left\lfloor \frac{n}{2} \right\rfloor - 2,\\
|E_{\{3,4\}}| &= |uv \in E(DA(T_n)) : d_u = 3 \ \textit{and} \ d_v = 4| = 1,\\
|E_{\{4,4\}}| &= |uv \in E(DA(T_n)) : d_u = 4 \ \textit{and} \ d_v = 4|\\
&= |E(DA(T_n))| - |E_{\{1,4\}}| - |E_{\{2,3\}}| - |E_{\{2,4\}}| - |E_{\{3,4\}}| = n - 3.
\end{aligned}$$

Thus, the $M-polynomial$ of $DA(T_n)$ is

$$\begin{aligned}
M(DA(T_n); x, y) &= \sum_{i \le j} m_{ij}(DA(T_n)) x^i y^j\\
&= \begin{cases} 4x^2y^3 + (4\left\lfloor \frac{n}{2} \right\rfloor - 4)x^2y^4 + 2x^3y^4 + (n-3)x^4y^4 & \textit{if } n \textit{ is even},\\ xy^4 + 2x^2y^3 + (4\left\lfloor \frac{n}{2} \right\rfloor - 2)x^2y^4 + x^3y^4 + (n-3)x^4y^4 & \textit{if } n \textit{ is odd}. \end{cases}
\end{aligned}$$

□

Definition 21. *The quadrilateral snake Q_n is obtained from the path P_n by replacing each edge of the path by a quadrilateral C_4.*

Theorem 2.26. *If Q_n is a quadrilateral snake, then*

$$M(Q_n; x, y) = 4x^2y^2 + 4(n-2)x^2y^4.$$

Proof. Let quadrilateral snake Q_n be a graph having $(3n-2)$ vertices and $4(n-1)$ edges. The edge partition of Q_n is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(Q_n) : d_u = 2 \ \textit{and} \ d_v = 2| = 4,\\
|E_{\{2,4\}}| &= |uv \in E(Q_n) : d_u = 2 \ \textit{and} \ d_v = 4|\\
&= |E(Q_n)| - |E_{\{2,2\}}| = 4(n-2).
\end{aligned}$$

Thus, the $M-polynomial$ of Q_n is

$$M(Q_n; x, y) = \sum_{i \le j} m_{ij}(Q_n) x^i y^j = 4x^2y^2 + 4(n-2)x^2y^4.$$

□

Definition 22. *A double quadrilateral snake DQ_n is a graph consisting two quadrilateral snakes that have a common path.*

Theorem 2.27. *If DQ_n is a double quadrilateral snake, then*

$$M(DQ_n; x, y) = 2(n-1)x^2y^2 + 4x^2y^3 + 4(n-2)x^2y^6 + 2x^3y^6 + (n-3)x^6y^6.$$

Proof. Let a double quadrilateral snake DQ_n be a graph having $(5n-4)$ vertices and $7(n-1)$ edges. The edge partition of DQ_n is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(DQ_n) : d_u = 2 \ \ and \ \ d_v = 2| = 2(n-1),\\
|E_{\{2,3\}}| &= |uv \in E(DQ_n) : d_u = 2 \ \ and \ \ d_v = 3| = 4,\\
|E_{\{2,6\}}| &= |uv \in E(DQ_n) : d_u = 2 \ \ and \ \ d_v = 6| = 4(n-2),\\
|E_{\{3,6\}}| &= |uv \in E(DQ_n) : d_u = 3 \ \ and \ \ d_v = 6| = 2,\\
|E_{\{6,6\}}| &= |uv \in E(DQ_n) : d_u = 6 \ \ and \ \ d_v = 6|\\
&= |E(DQ_n)| - |E_{\{2,2\}}| - |E_{\{2,3\}}| - |E_{\{2,6\}}| - |E_{\{3,6\}}| = n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of DQ_n is

$$M(DQ_n;x,y) = \sum_{i\le j} m_{ij}(DQ_n)x^iy^j = 2(n-1)x^2y^2+4x^2y^3+4(n-2)x^2y^6+2x^3y^6+(n-3)x^6y^6.$$

□

Definition 23. *The alternate quadrilateral snake $A(Q_n)$ is obtained from a path $v_1v_2...v_n$ by joining v_i, v_{i+1} (alternatively) to new vertices v_i, w_i respectively and then joining v_i and w_i. i.e., every alternate edge of a path is replaced by a cycle C_4.*

Theorem 2.28. *If $A(Q_n)$ is an alternate quadrilateral snake, then*

$$M(A(Q_n);x,y) = \begin{cases} \left(\frac{n}{2}+2\right)x^2y^2 + nx^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is even},\\ xy^3 + \left(\lfloor\frac{n}{2}\rfloor+1\right)x^2y^2 + 2\lfloor\frac{n}{2}\rfloor x^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is odd}. \end{cases}$$

Proof. Let an alternate quadrilateral snake $A(Q_n)$ be a graph having $(n+2\lfloor\frac{n}{2}\rfloor)$ vertices and $(3\lfloor\frac{n}{2}\rfloor+n-1)$ edges. The edge partition of $A(Q_n)$ is given as follows: If n is even, then there will be no pendant edge in $A(T_n)$. Therefore, we have

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(A(Q_n)) : d_u = 2 \ \ and \ \ d_v = 2| = \frac{n}{2}+2,\\
|E_{\{2,3\}}| &= |uv \in E(A(Q_n)) : d_u = 2 \ \ and \ \ d_v = 3| = n,\\
|E_{\{3,3\}}| &= |uv \in E(A(Q_n)) : d_u = 3 \ \ and \ \ d_v = 3|\\
&= |E(A(Q_n))| - |E_{\{2,2\}}| - |E_{\{2,3\}}| = n-3.
\end{aligned}$$

If n is odd, then there will be a pendant edge in $A(T_n)$. Therefore, we have

$$\begin{aligned}
|E_{\{1,3\}}| &= |uv \in E(A(Q_n)) : d_u = 1 \ \ and \ \ d_v = 3| = 1,\\
|E_{\{2,2\}}| &= |uv \in E(A(Q_n)) : d_u = 2 \ \ and \ \ d_v = 2| = \left\lfloor\frac{n}{2}\right\rfloor+1,\\
|E_{\{2,3\}}| &= |uv \in E(A(Q_n)) : d_u = 2 \ \ and \ \ d_v = 3| = 2\left\lfloor\frac{n}{2}\right\rfloor,\\
|E_{\{3,3\}}| &= |uv \in E(A(Q_n)) : d_u = 3 \ \ and \ \ d_v = 3|\\
&= |E(A(Q_n))| - |E_{\{1,3\}}| - |E_{\{2,2\}}| - |E_{\{2,3\}}| = n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of $A(Q_n)$ is

$$\begin{aligned}
M(A(Q_n);x,y) &= \sum_{i\le j} m_{ij}(A(Q_n))x^iy^j\\
&= \begin{cases} \left(\frac{n}{2}+2\right)x^2y^2 + nx^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is even},\\ xy^3 + \left(\lfloor\frac{n}{2}\rfloor+1\right)x^2y^2 + 2\lfloor\frac{n}{2}\rfloor x^2y^3 + (n-3)x^3y^3 & \text{if } n \text{ is odd}. \end{cases}
\end{aligned}$$

□

Definition 24. *An irregular quadrilateral snake* IQ_n *is a graph obtained from the path* $P_n : u_1u_2...u_n$ *with vertex set* $V(IQ_n) = V(P_n) \cup \{v_i, w_i : 1 \leq i \leq n-2\}$ *and the edge set* $E(IQ_n) = E(P_n) \cup \{u_iv_i, w_iu_{i+2} : 1 \leq i \leq n-2\}$.

Theorem 2.29. *If* IQ_n *is an irregular quadrilateral snake, then*

$$M(IQ_n; x, y) = nx^2y^2 + 4x^2y^3 + 2(n-4)x^2y^4 + 2x^3y^4 + (n-5)x^4y^4.$$

Proof. Let an irregular quadrilateral snake IQ_n be a graph having $(3n-4)$ vertices and $(4n-7)$ edges. The edge partition of IQ_n is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(IQ_n) : d_u = 2 \;\; and \;\; d_v = 2| = n, \\
|E_{\{2,3\}}| &= |uv \in E(IQ_n) : d_u = 2 \;\; and \;\; d_v = 3| = 4, \\
|E_{\{2,4\}}| &= |uv \in E(IQ_n) : d_u = 2 \;\; and \;\; d_v = 4| = 2(n-4), \\
|E_{\{3,4\}}| &= |uv \in E(IQ_n) : d_u = 3 \;\; and \;\; d_v = 4| = 2, \\
|E_{\{4,4\}}| &= |uv \in E(IQ_n) : d_u = 4 \;\; and \;\; d_v = 4| \\
&= |E(IQ_n)| - |E_{\{2,2\}}| - |E_{\{2,3\}}| - |E_{\{2,4\}}| - |E_{\{3,4\}}| = n-5.
\end{aligned}$$

Thus, the $M-polynomial$ of IQ_n is

$$M(IQ_n; x, y) = \sum_{i \leq j} m_{ij}(IQ_n)x^iy^j = nx^2y^2 + 4x^2y^3 + 2(n-4)x^2y^4 + 2x^3y^4 + (n-5)x^4y^4.$$

□

Definition 25. *A double alternate quadrilateral snake* $DA(Q_n)$ *consists of two alternate quadrilateral snakes that have a common path.*

Theorem 2.30. *If* $DA(Q_n)$ *is a double alternate quadrilateral snake, then*

$$M(DA(Q_n); x, y) = \begin{cases} nx^2y^2 + 4x^2y^3 + 2(n-2)x^2y^4 + 2x^3y^4 + (n-3)x^4y^4 & \textit{if n is even,} \\ xy^4 + 2\lfloor \frac{n}{2} \rfloor x^2y^2 + 2x^2y^3 + 2(n-2)x^2y^4 + x^3y^4 + (n-3)x^4y^4 & \textit{if n is odd.} \end{cases}$$

Proof. Let a double alternate quadrilateral snake $DA(Q_n)$ be a graph having $(n + 4\lfloor \frac{n}{2} \rfloor)$ vertices and $(6\lfloor \frac{n}{2} \rfloor + n - 1)$ edges. The edge partition of $DA(Q_n)$ is given as follows:
If n is even, then there will be no pendant edge in $DA(T_n)$. Therefore, we have

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(DA(Q_n)) : d_u = 2 \;\; and \;\; d_v = 2| = n, \\
|E_{\{2,3\}}| &= |uv \in E(DA(Q_n)) : d_u = 2 \;\; and \;\; d_v = 3| = 4, \\
|E_{\{2,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 2 \;\; and \;\; d_v = 4| = 2(n-2), \\
|E_{\{3,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 3 \;\; and \;\; d_v = 4| = 2, \\
|E_{\{4,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 4 \;\; and \;\; d_v = 4| \\
&= |E(DA(Q_n))| - |E_{\{2,2\}}| - |E_{\{2,3\}}| - |E_{\{2,4\}}| - |E_{\{3,4\}}| = n-3.
\end{aligned}$$

If n is odd, then there will be a pendant edge in $DA(T_n)$. Therefore, we have

$$\begin{aligned}
|E_{\{1,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 1 \ \ and \ \ d_v = 4| = 1, \\
|E_{\{2,2\}}| &= |uv \in E(DA(Q_n)) : d_u = 2 \ \ and \ \ d_v = 2| = 2\left\lfloor \frac{n}{2} \right\rfloor, \\
|E_{\{2,3\}}| &= |uv \in E(DA(Q_n)) : d_u = 2 \ \ and \ \ d_v = 3| = 2, \\
|E_{\{2,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 2 \ \ and \ \ d_v = 4| = 2(n-2), \\
|E_{\{3,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 3 \ \ and \ \ d_v = 4| = 1, \\
|E_{\{4,4\}}| &= |uv \in E(DA(Q_n)) : d_u = 4 \ \ and \ \ d_v = 4| \\
&= |E(DA(Q_n))| - |E_{\{1,4\}}| - |E_{\{2,2\}}| - |E_{\{2,3\}}| - |E_{\{2,4\}}| - |E_{\{3,4\}}| = n-3.
\end{aligned}$$

Thus, the $M-polynomial$ of $DA(Q_n)$ is

$$\begin{aligned}
M(DA(Q_n); x, y) &= \sum_{i \le j} m_{ij}(DA(Q_n)) x^i y^j \\
&= \begin{cases} nx^2y^2 + 4x^2y^3 + 2(n-2)x^2y^4 + 2x^3y^4 + (n-3)x^4y^4 & if\ n\ is\ even, \\ xy^4 + 2\lfloor \frac{n}{2} \rfloor x^2y^2 + 2x^2y^3 + 2(n-2)x^2y^4 + x^3y^4 + (n-3)x^4y^4 & if\ n\ is\ odd. \end{cases}
\end{aligned}$$

□

Definition 26. *The graph DW_n is a graph consisting of the two wheels W_n of the same order having the same central vertex.*

Theorem 2.31. *If DW_n is a graph with $(2n+1)$ vertices and $4n$ edges, then*

$$M(DW_n; x, y) = 2nx^3y^3 + 2nx^3y^{2n}.$$

Proof. Let DW_n be a graph having $(2n+1)$ vertices and $4n$ edges. The edge partition of DW_n is given by,

$$\begin{aligned}
|E_{\{3,3\}}| &= |uv \in E(DW_n) : d_u = 3 \ \ and \ \ d_v = 3| = 2n, \\
|E_{\{3,2n\}}| &= |uv \in E(DW_n) : d_u = 3 \ \ and \ \ d_v = 2n| \\
&= |E(DW_n)| - |E_{\{3,3\}}| = 2n.
\end{aligned}$$

Thus, the $M-polynomial$ of DW_n is

$$M(DW_n; x, y) = \sum_{i \le j} m_{ij}(DW_n) x^i y^j = 2nx^3y^3 + 2nx^3y^{2n}.$$

□

Definition 27. *The AC_n be a graph obtained from a cycle $C_n : u_1u_2...u_nu_1$ with the vertex set $V(AC_n) = V(C_n) \cup \{v_i, w_i : 1 \le i \le n\}$ and the edge set $E(AC_n) = E(C_n) \cup \{u_iv_i, v_iw_i : 1 \le i \le n\}$.*

Theorem 2.32. *If AC_n is a graph with $3n$ vertices and $3n$ edges, then*

$$M(AC_n; x, y) = nxy^2 + nx^2y^3 + nx^3y^3.$$

Proof. Let AC_n is a graph having $3n$ vertices and $3n$ edges. The edge partition of AC_n is given by,

$$\begin{aligned}
|E_{\{1,2\}}| &= |uv \in E(AC_n) : d_u = 1 \ \ and \ \ d_v = 2| = n, \\
|E_{\{2,3\}}| &= |uv \in E(AC_n) : d_u = 2 \ \ and \ \ d_v = 3| = n, \\
|E_{\{3,3\}}| &= |uv \in E(AC_n) : d_u = 3 \ \ and \ \ d_v = 3| \\
&= |E(AC_n)| - |E_{\{1,2\}}| - |E_{\{2,3\}}| = n.
\end{aligned}$$

Thus, the $M-polynomial$ of AC_n is

$$M(AC_n;x,y)=\sum_{i\le j}m_{ij}(AC_n)x^iy^j=nxy^2+nx^2y^3+nx^3y^3.$$

□

Definition 28. *An umbrella* $U_{m,n}=(P_m+K_1)\circ P_n$ *is a graph of order* $(m+n)$ *and size* $(2m+n-2)$*, where* P_m *and* P_n *are the two paths of lengths* $(m-1)$ *and* $(n-1)$*, respectively.*

Theorem 2.33. *If* $U_{m,n}$ *is an umbrella with* $(m+n)$ *vertices and* $(2m+n-2)$ *edges, then*

$$M(U_{m,n};x,y)=xy^2+(n-3)x^2y^2+2x^2y^3+3x^2y^{m+1}+(m-3)x^3y^3+(m-2)x^3y^{m+1}.$$

Proof. Let an umbrella $U_{m,n}$ be a graph having $(m+n)$ vertices and $(2m+n-2)$ edges. The edge partition of $U_{m,n}$ is given by,

$$\begin{aligned}
|E_{\{1,2\}}| &= |uv\in E(U_{m,n}):d_u=1 \ \ and \ \ d_v=2|=1,\\
|E_{\{2,2\}}| &= |uv\in E(U_{m,n}):d_u=2 \ \ and \ \ d_v=2|=n-3,\\
|E_{\{2,3\}}| &= |uv\in E(U_{m,n}):d_u=2 \ \ and \ \ d_v=3|=2,\\
|E_{\{2,m+1\}}| &= |uv\in E(U_{m,n}):d_u=2 \ \ and \ \ d_v=m+1|=3,\\
|E_{\{3,3\}}| &= |uv\in E(U_{m,n}):d_u=3 \ \ and \ \ d_v=3|=m-3,\\
|E_{\{3,m+1\}}| &= |uv\in E(U_{m,n}):d_u=3 \ \ and \ \ d_v=m+1|\\
&= |E(U_{m,n})|-|E_{\{1,2\}}|-|E_{\{2,2\}}|-|E_{\{2,3\}}|-|E_{\{2,m+1\}}|-|E_{\{3,3\}}|=m-2.
\end{aligned}$$

Thus, the $M-polynomial$ of $U_{m,n}$ is

$$M(U_{m,n};x,y)=\sum_{i\le j}m_{ij}(U_{m,n})x^iy^j=xy^2+(n-3)x^2y^2+2x^2y^3+3x^2y^{m+1}+(m-3)x^3y^3+(m-2)x^3y^{m+1}.$$

□

Definition 29. *A Dumbbell* Db_n *is a graph obtained from two cycles of length* n *by joining a vertex from one cycle to a vertex of another cycle.*

Theorem 2.34. *If* Db_n *is a dumbbell with* $2n$ *vertices and* $(2n+1)$ *edges, then*

$$M(Db_n;x,y)=2(n-2)x^2y^2+4x^2y^3+x^3y^3.$$

Proof. Let a dumbbell Db_n be a graph having $2n$ vertices and $(2n+1)$ edges. The edge partition of Db_n is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv\in E(Db_n):d_u=2 \ \ and \ \ d_v=2|=2(n-2),\\
|E_{\{2,3\}}| &= |uv\in E(Db_n):d_u=2 \ \ and \ \ d_v=3|=4,\\
|E_{\{3,3\}}| &= |uv\in E(Db_n):d_u=3 \ \ and \ \ d_v=3|\\
&= |E(Db_n)|-|E_{\{2,2\}}|-|E_{\{2,3\}}|=1.
\end{aligned}$$

Thus, the $M-polynomial$ of Db_n is

$$M(Db_n;x,y)=\sum_{i\le j}m_{ij}(Db_n)x^iy^j=2(n-2)x^2y^2+4x^2y^3+x^3y^3.$$

□

Definition 30. *The slanting ladder* SL_n *is a graph obtained from two paths* $u_1u_2...u_n$ *and* $v_1v_2...v_n$ *by joining each* u_i *with* $v_{i+1}, (1\le i\le n-1)$.

Theorem 2.35. *If SL_n is a slanting ladder with $2n$ vertices and $3(n-1)$ edges, then*

$$M(SL_n; x, y) = 2xy^3 + 4x^2y^3 + 3(n-3)x^3y^3.$$

Proof. Let a slanting ladder SL_n be a graph having $2n$ vertices and $3(n-1)$ edges. The edge partition of SL_n is given by,

$$\begin{aligned}
|E_{\{1,3\}}| &= |uv \in E(SL_n) : d_u = 1 \;\; and \;\; d_v = 3| = 2, \\
|E_{\{2,3\}}| &= |uv \in E(SL_n) : d_u = 2 \;\; and \;\; d_v = 3| = 4, \\
|E_{\{3,3\}}| &= |uv \in E(SL_n) : d_u = 3 \;\; and \;\; d_v = 3| \\
&= |E(SL_n)| - |E_{\{1,3\}}| - |E_{\{2,3\}}| = 3(n-3).
\end{aligned}$$

Thus, the $M-polynomial$ of SL_n is

$$M(SL_n; x, y) = \sum_{i \le j} m_{ij}(SL_n)x^iy^j = 2xy^3 + 4x^2y^3 + 3(n-3)x^3y^3.$$

□

Definition 31. *The triangular ladder TL_n with vertex set $V(TL_n) = \{u_i, v_i : 1 \le i \le n\}$ and the edge set $E(TL_n) = \{u_iu_{i+1}, v_iv_{i+1}, u_iv_{i+1} : 1 \le i \le n\} \cup \{u_iv_i : 1 \le i \le n\}$.*

Theorem 2.36. *If TL_n is a triangular ladder with $2n$ vertices and $(4n-3)$ edges, then*

$$M(TL_n; x, y) = 2x^2y^3 + 2x^2y^4 + 4x^3y^4 + (4n-11)x^4y^4.$$

Proof. Let a triangular ladder TL_n be a graph having $2n$ vertices and $(4n-3)$ edges. The edge partition of TL_n is given by,

$$\begin{aligned}
|E_{\{2,3\}}| &= |uv \in E(TL_n) : d_u = 2 \;\; and \;\; d_v = 3| = 2, \\
|E_{\{2,4\}}| &= |uv \in E(TL_n) : d_u = 2 \;\; and \;\; d_v = 4| = 2, \\
|E_{\{3,4\}}| &= |uv \in E(TL_n) : d_u = 3 \;\; and \;\; d_v = 4| = 4, \\
|E_{\{4,4\}}| &= |uv \in E(TL_n) : d_u = 4 \;\; and \;\; d_v = 4| \\
&= |E(TL_n)| - |E_{\{2,3\}}| - |E_{\{2,4\}}| - |E_{\{3,4\}}| = (4n-11).
\end{aligned}$$

Thus, the $M-polynomial$ of TL_n is

$$M(TL_n; x, y) = \sum_{i \le j} m_{ij}(TL_n)x^iy^j = 2x^2y^3 + 2x^2y^4 + 4x^3y^4 + (4n-11)x^4y^4.$$

□

Definition 32. *The n-cone graph $C_m + \overline{K_n}$ is a graph where C_m is a cycle of order m and K_n is a complete graph of order n.*

Theorem 2.37. *If $C_m + \overline{K_n}$ is a n-cone with $(m+n)$ vertices and $m(n+1)$ edges, then*

$$M(C_m + \overline{K_n}; x, y) = mnx^my^{n+2} + mx^{n+2}y^{n+2}.$$

Proof. Let a n-cone graph $C_m + \overline{K_n}$ be a graph having $(m+n)$ vertices and $m(n+1)$ edges. The edge partition of $C_m + \overline{K_n}$ is given by,

$$\begin{aligned}
|E_{\{m,n+2\}}| &= |uv \in E(C_m + \overline{K_n}) : d_u = m \;\; and \;\; d_v = n+2| = mn, \\
|E_{\{n+2,n+2\}}| &= |uv \in E(C_m + \overline{K_n}) : d_u = n+2 \;\; and \;\; d_v = n+2| \\
&= |E(C_m + \overline{K_n})| - |E_{\{m,n+2\}}| = m.
\end{aligned}$$

Thus, the $M-polynomial$ of $C_m+\overline{K_n}$ is

$$M(C_m+\overline{K_n};x,y)=\sum_{i\le j} m_{ij}(C_m+\overline{K_n})x^iy^j=mnx^my^{n+2}+mx^{n+2}y^{n+2}.$$

□

Definition 33. *The graph* $C_n^{+(m,t)}$ *is obtained by identifying one vertex of* C_n *with one end vertex of* m *paths each of length* t. *In particular,* $C_n^{+(1,t)}$ *is a tadpole.*

Theorem 2.38. *If* $C_n^{+(m,t)}$ *is a graph with* $(n+t)$ *vertices and* $(mt+n)$ *edges, then*

$$M(C_n^{+(m,t)};x,y)=mxy^2+(m+n-2)x^2y^2+(m+2)x^2y^{m+2}.$$

Proof. Let $C_n^{+(m,t)}$ be a graph having $(n+t)$ vertices and $(mt+n)$ edges. The edge partition of $C_n^{+(m,t)}$ is given by,

$$\begin{aligned}|E_{\{1,2\}}| &= |uv\in E(C_n^{+(m,t)}):d_u=1 \ \ and \ \ d_v=2|=m,\\ |E_{\{2,2\}}| &= |uv\in E(C_n^{+(m,t)}):d_u=2 \ \ and \ \ d_v=2|=m+n-2,\\ |E_{\{2,m+2\}}| &= |uv\in E(C_n^{+(m,t)}):d_u=2 \ \ and \ \ d_v=m+2|\\ &= |E(C_n^{+(m,t)})|-|E_{\{1,2\}}|-|E_{\{2,2\}}|=m+2.\end{aligned}$$

Thus, the $M-polynomial$ of $C_n^{+(m,t)}$ is

$$M(C_n^{+(m,t)};x,y)=\sum_{i\le j} m_{ij}(C_n^{+(m,t)})x^iy^j=mxy^2+(m+n-2)x^2y^2+(m+2)x^2y^{m+2}.$$

□

Definition 34. *The graph* $\theta(C_m)^n$ *is obtained from* n *copies of* C_m *that shares an edge in common, where* C_m *is a cycle of length* m. *i.e., an* n *page book graph with* m*-polygonal pages.*

Theorem 2.39. *If* $\theta(C_m)^n$ *is an* n *page book graph with* m*-polygonal pages, then*

$$M(\theta(C_m)^n;x,y)=n(m-3)x^2y^2+2nx^2y^{n+1}+x^{n+1}y^{n+1}.$$

Proof. Let $\theta(C_m)^n$ be a graph having $n(m-2)+2$ vertices and $n(m-1)+1$ edges. The edge partition of $\theta(C_m)^n$ is given by,

$$\begin{aligned}|E_{\{2,2\}}| &= |uv\in E(\theta(C_m)^n):d_u=2 \ \ and \ \ d_v=2|=n(m-3),\\ |E_{\{2,n+1\}}| &= |uv\in E(\theta(C_m)^n):d_u=2 \ \ and \ \ d_v=n+1|=2n,\\ |E_{\{n+1,n+1\}}| &= |uv\in E(\theta(C_m)^n):d_u=n+1 \ \ and \ \ d_v=n+1|\\ &= |E(\theta(C_m)^n)|-|E_{\{2,2\}}|-|E_{\{2,n+1\}}|=1.\end{aligned}$$

Thus, the $M-polynomial$ of $\theta(C_m)^n$ is

$$M(\theta(C_m)^n;x,y)=\sum_{i\le j} m_{ij}(\theta(C_m)^n)x^iy^j=n(m-3)x^2y^2+2nx^2y^{n+1}+x^{n+1}y^{n+1}.$$

□

Definition 35. *The kayak paddle graph* $KP(k,m,l)$ *is a graph obtained by joining two cycles* C_k *and* C_m *by a path of length* l.

Theorem 2.40. *If* $KP(k,m,l)$ *is a kayak paddle graph, then*

$$M(KP(k,m,l);x,y)=(k+m+l-6)x^2y^2+6x^2y^3.$$

Proof. Let $KP(k,m,l)$ be a graph having $(k+m+l-1)$ vertices and $(k+m+l)$ edges. The edge partition of $KP(k,m,l)$ is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(KP(k,m,l)) : d_u = 2 \ \ and \ \ d_v = 2| = k+m+l-6, \\
|E_{\{2,3\}}| &= |uv \in E(KP(k,m,l)) : d_u = 2 \ \ and \ \ d_v = 3| \\
&= |E(KP(k,m,l))| - |E_{\{2,2\}}| = 6.
\end{aligned}$$

Thus, the $M - polynomial$ of $KP(k,m,l)$ is

$$M(KP(k,m,l);x,y) = \sum_{i \le j} m_{ij}(KP(k,m,l))x^i y^j = (k+m+l-6)x^2y^2 + 6x^2y^3.$$

□

Definition 36. *The graph $C_n^{(t)}$ is obtained from the one-point union of t cycles of length n.*

Theorem 2.41. *If $C_n^{(t)}$ is a graph with $t(n-1)+1$ vertices and nt edges, then*

$$M(C_n^{(t)};x,y) = t(n-2)x^2y^2 + 2tx^2y^{2t}.$$

Proof. Let $C_n^{(t)}$ be a graph having $t(n-1)+1$ vertices and nt edges. The edge partition of $C_n^{(t)}$ is given by,

$$\begin{aligned}
|E_{\{2,2\}}| &= |uv \in E(C_n^{(t)}) : d_u = 2 \ \ and \ \ d_v = 2| = t(n-2), \\
|E_{\{2,2t\}}| &= |uv \in E(C_n^{(t)}) : d_u = 2 \ \ and \ \ d_v = 2t| \\
&= |E(C_n^{(t)})| - |E_{\{2,2\}}| = 2t.
\end{aligned}$$

Thus, the $M - polynomial$ of $C_n^{(t)}$ is

$$M(C_n^{(t)};x,y) = \sum_{i \le j} m_{ij}(C_n^{(t)})x^i y^j = t(n-2)x^2y^2 + 2tx^2y^{2t}.$$

□

Note that, the topological indices (that are mentioned in Table 1) of all these special graphs can be obtained by using respective $M-$polynomial and column 4 of Table 1. The process of obtaining these topological indices is given in two Corollaries 2.11 and 2.13 as an illustration.

3. CONCLUSION

In this paper, we have obtained M-polynomial of some special graphs and some topological indices of these graphs. The advantage of M-polynomial is that, from that one expression we can obtain several degree-based topological indices. It is very challenging to bring all the degree-based topological indices under $M-$polynomial.

4. ACKNOWLEDGEMENT

The authors are thankful to the referee for useful suggestions. The first author is thankful to University Grants Commission (UGC), Government of India, New Delhi, for the financial support through UGC-SAP DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I) dated: 29th Feb. 2016. The second author is thankful to Directorate of Minorities, Government of Karnataka, Bangalore, for the financial support through M. Phil/Ph. D. Fellowship 2017-18: No.DOM/FELLOWSHIP/CR-29/2017-18 dated: 09th Aug. 2017.

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International Journal of Scientific Research in Mathematical and Statistical Sciences
Volume-6, Issue-2, pp.80-84, April (2019)

Research Paper

E-ISSN: 2348-4519

Computation of leap hyper-Zagreb indices of certain windmill graphs

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Available online at: www.isroset.org

Received …. 2019, Accepted: 14/Apr/2019, Online: 31/Apr/2019

***Abstract*—** In this paper, we establish the expressions for the first and second leap hyper-Zagreb indices of certain windmill graphs such as French windmill graph $\boldsymbol{F_n^m}$, Dutch windmill graph $\boldsymbol{D_n^m}$, Kulli cycle windmill graph $\boldsymbol{C_{n+1}^m}$ and Kulli path windmill graph $\boldsymbol{P_{n+1}^m}$.

Keywords— *French Windmill graph; Dutch Windmill graph; Kulli cycle windmill graph; Kulli path windmill graph; leap hyper-Zagreb index.*

I. INTRODUCTION

Throughout this paper, we consider only finite, connected, undirected graphs without loops and multiple edges. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex v, the degree $d(v)$ is the number of vertices adjacent to v. The distance $d(u,v)$ between any two vertices u and v is the length of shortest path connecting u and v. For a positive integer k, the open k-neighbourhood $N_k(v)$ of a vertex v in a graph G is defined as $N_k(v/G) = \{u \in V(G): d(u,v) = k\}$. The k-distance degree $d_k(v)$ of a vertex v in G is defined as the number of k neighbours of v in G. We denote $d_k(v) = |N_k(v)|$. We refer to [10] for undefined terminologies and notations from graph theory.

A topological index is a numerical parameter mathematically derived from the graph structure. It is a graph invariant. The topological indices have their applications in various disciplines of science and technology. The first and second Zagreb indices are amongst the oldest and best known topological indices defined in 1972 by Gutman [7] as follows:

$$M_1(G) = \sum_{v \in V(G)} d(v)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d(u) \cdot d(v),$$

respectively.

In 2017, Naji et al. [8] defined first and second leap Zagreb indices by taking 2-distance degree of vertices instead of taking vertex degree and they are defined as follows:

$$LM_1(G) = \sum_{v \in V(G)} d_2(v)^2$$

and

$$LM_2(G) = \sum_{uv \in E(G)} d_2(u) \cdot d_2(v),$$

respectively. For more details one can refer to [1,2,4,5,9].

A new version of the first leap Zagreb index was proposed by Kulli in [13], defined as

$$LM_1^*(G) = \sum_{uv \in E(G)} [d_2(u) + d_2(v)]. \qquad (1.1)$$

The first and second leap hyper-Zagreb indices were introduced in [13] and they are defined as

$$HLM_1(G) = \sum_{uv \in E(G)} [d_2(u) + d_2(v)]^2, \qquad (1.2)$$

and

$$HLM_2(G) = \sum_{uv \in E(G)} [d_2(u) \cdot d_2(v)]^2 \qquad (1.3)$$

respectively. For applications of first and second leap hyper-Zagreb indices one can refer [3].

The rest of the paper is organized as follows. In sections II, III, IV and V, we obtain the expressions for first, second leap hyper-Zagreb indices of french windmill graphs, dutch windmill graphs, Kulli cycle windmill graphs and Kulli path windmill graphs, respectively.

II. FRENCH WINDMILL GRAPHS

The French windmill graph [6] F_n^m is the graph obtained by taking $m \geq 2$ copies of $K_n, n \geq 2$ with a vertex in common. The graph F_n^m is shown in Figure 1. The French windmill graph F_2^m is called a star graph, the French windmill graph F_3^m is called a friendship graph and the French windmill graph F_4^2 is called a butterfly graph.

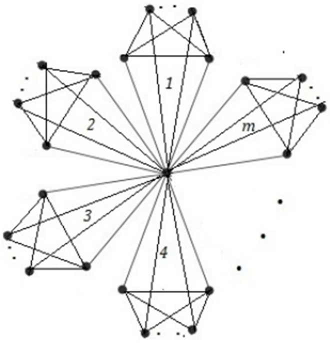

Figure 1: French windmill graph F_n^m

Let F be a French windmill graph F_n^m. The graph has $1+m(n-1)$ vertices and $\frac{1}{2}mn(n-1)$ edges, $m \geq 2, n \geq 2$. Then there are two types of the 2-distance degree of edges as given in Table 1.

Table 1: 2-distance degree edge partition of F

$d_2(u), d_2(v) \mid uv \in E(F)$	$(0, (n-1)(m-1))$	$((n-1)(m-1), (n-1)(m-1))$
Number of edges	$m(n-1)$	$\frac{1}{2}m(n-1)(n-2)$

Theorem 2.1. *The new version of first leap Zagreb index of a French windmill graph F_n^m is given by*

$$LM_1^*(F_n^m) \quad = \quad m(m-1)(n-1)^3.$$

Proof. Let $F = F_n^m$. From Eq. (1.1) and by using Table 1, we obtain

$$\begin{aligned} LM_1^*(F_n^m) &= \sum_{uv \in E(F)} [d_2(u) + d_2(v)] \\ &= [0 + (n-1)(m-1)]m(n-1) \\ &\quad + \frac{1}{2}[(n-1)(m-1) + (n-1)(m-1)]m(n \\ &\quad - 1)(n-2) \\ &= m(m-1)(n-1)^3. \end{aligned}$$

Theorem 2.2. *The first leap hyper-Zagreb index of a French windmill graph F_n^m is*

$$HLM_1(F_n^m) = m(m-1)^2(n-1)^3(2n-3).$$

Proof. Let F be the graph of a French windmill graph F_n^m. By using Eq. (1.2) and by using Table 1, we deduce

$$\begin{aligned} HLM_1(F_n^m) &= \sum_{uv \in E(F)} [d_2(u) + d_2(v)]^2 \\ &= [0 + (n-1)(m-1)]^2 m(n-1) \\ &\quad + \frac{1}{2}[(n-1)(m-1) + (n-1)(m-1)]^2 m(n \\ &\quad - 1)(n-2) \\ &= m(m-1)^2\,(n-1)^3(2n-3). \end{aligned}$$

Theorem 2.3. *The second leap hyper-Zagreb index of F_n^m is*

$$HLM_2(F_n^m) = \frac{1}{2}m(m-1)^4(n-1)^5(n-2).$$

Proof. Let $F = F_n^m$. From Eq. (1.3), we have

$$HLM_2(F_n^m) \quad = \quad \sum_{uv \in E(F)} [d_2(u)d_2(v)]^2$$

By using Table 1, we derive

$$\begin{aligned} HLM_2(F_n^m) &= [0 \times (n-1)(m-1)]^2 m(n-1) \\ &\quad + \frac{1}{2}[(n-1)(m-1) \times (n-1)(m-1)]^2 m(n \\ &\quad - 1)(n-2) \\ &= \frac{1}{2}m(m-1)^4(n-1)^5(n-2). \end{aligned}$$

III. DUTCH WINDMILL GRAPHS

The Dutch windmill graph, denoted by $D_n^m, m \geq 2, n \geq 5$, is the graph obtained by taking m copies of C_n with a vertex in common. The graph D_n^m is presented in Figure 2. The dutch windmill graph D_3^m is called a friendship graph. For more details on windmill graph, see [6].

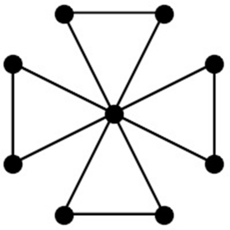

Figure 2: Dutch windmill graph D_3^4

Let D be a Dutch windmill graph D_n^m. The graph has $1+m(n-1)$ vertices and mn edges, $m \geq 2, n \geq 5$. Then the edge partitions of 2-distance degree of edges as given in Table 2.

Table 2: 2-distance degree edge partition of D

$d_2(u), d_2(v) \mid uv \in E(D)$	$(2m, 2m)$	$(2m, 2)$	$(2,2)$
Number of edges	$2m$	$2m$	$m(n-4)$

Theorem 3.1. *Let D be the graph of a Dutch windmill graph* D_n^m. *Then*

$$LM_1^*(D_n^m) \quad = \quad 4mn + 12m^2 - 12m.$$

Proof. By using Eq. (1.1) and Table 2, we obtain

$$\begin{aligned} LM_1^*(D_n^m) &= \sum_{uv \in E(D)} [d_2(u) + d_2(v)] \\ &= (2m + 2m)2m + (2m + 2)2m + (2 + 2)m(n-4) \\ &= 4mn + 12m^2 - 12m. \end{aligned}$$

Theorem 3.2. *The first leap hyper-Zagreb index of Dutch windmill graph* D_n^m *is given by*

$$HLM_1(D_n^m) = 16mn + 40m^3 + 16m^2 - 56m.$$

Proof. Let D be the graph of a Dutch windmill graph D_n^m. By using Eq. (1.2) and by using Table 2, we derive

$$\begin{aligned} HLM_1(D_n^m) &= \sum_{uv \in E(D)} [d_2(u) + d_2(v)]^2 \\ &= (2m + 2m)^2 2m + (2m + 2)^2 2m + (2 + 2)^2 m(n-4) \\ &= 16mn + 40m^3 + 16m^2 - 56m. \end{aligned}$$

Theorem 3.3. *The second leap hyper-Zagreb index of Dutch windmill graph* D_n^m *is*

$$HLM_2(D_n^m) = 16mn + 36m^5 + 32m^3 - 64m.$$

Proof. Let $D = D_n^m$. By using Eq. (1.3), we have

$$HLM_2(D_n^m) \quad = \quad \sum_{uv \in E(D)} [d_2(u) d_2(v)]^2$$

By using Table 2, we deduce

$$\begin{aligned} HLM_2(D_n^m) &= (2m + 2m)^2 2m + (2m + 2)^2 2m \\ &\quad + (2 + 2)^2 m(n-4) \\ &= 16mn + 36m^5 + 32m^3 - 64m. \end{aligned}$$

IV. KULLI CYCLE WINDMILL GRAPHS

The Kulli cycle windmill graph [11] is the graph obtained by taking m copies of the graph $K_1 + C_n$ for $n \geq 3$ with a vertex K_1 in common and it is denoted by C_{n+1}^m This graph is depicted in Figure 3.

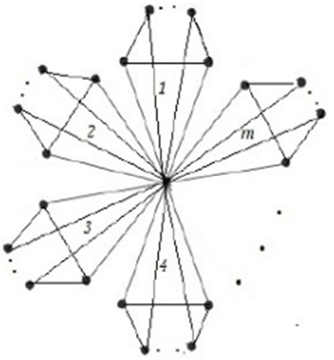

Figure 3: Kulli cycle windmill graph C_{n+1}^m.

Let $C = C_{n+1}^m$ be a Kulli cycle windmill graph with $mn + 1$ vertices and $2mn$ edges, $m \geq 2, n \geq 5$. Then C has two types of 2-distance degree of edges as given in Table 3.

Table 3: 2-distance degree edge partition of C

$d_2(u), d_2(v) \mid uv \in E(C)$	$(0, mn-3)$	$(mn-3, mn-3)$
Number of edges	mn	mn

Theorem 4.1. *Let* $C = C_{n+1}^m, m \geq 2, n \geq 5$. *Then*

$$LM_1^*(C_{n+1}^m) \quad = \quad 3mn(mn-3).$$

Proof. From Eq. (1.1) and using Table 3, we obtain

$$\begin{aligned} LM_1^*(C_{n+1}^m) &= \sum_{uv \in E(C)} [d_2(u) + d_2(v)] \\ &= (0 + mn - 3)mn + (mn - 3 + mn - 3)mn \\ &= 3mn(mn-3). \end{aligned}$$

Theorem 4.2. *The first leap hyper-Zagreb index of* C_{n+1}^m *is given by*

$$HLM_1(C_{n+1}^m) = 5mn(mn-3)^2.$$

Proof. By using Eq. (1.2) and by using Table 3, we derive

$$\begin{aligned} HLM_1(C_{n+1}^m) &= \sum_{uv \in E(C)} [d_2(u) + d_2(v)]^2 \\ &= (0 + mn - 3)^2 mn + (mn - 3 + mn - 3)^2 mn \\ &= 5mn(mn-3)^2. \end{aligned}$$

Theorem 4.3. *The second leap hyper-Zagreb index of Dutch windmill graph* C_{n+1}^m *is*

$$HLM_2(C_{n+1}^m) = mn(mn-3)^4.$$

Proof. By using Eq. (1.3), we have

$$HLM_2(C_{n+1}^m) \quad = \quad \sum_{uv\in E(C)} [d_2(u)d_2(v)]^2$$

By using Table 3, we obtain

$$\begin{aligned} HLM_2(C_{n+1}^m) &= (0\times(mn-3))^2 mn \\ &\quad +((mn-3)(mn-3))^2 mn \\ &= mn(mn-3)^4. \end{aligned}$$

V. KULLI PATH WINDMILL GRAPHS

The Kulli path windmill graph [12] is the graph obtained by taking m copies of the graph $K_1 + P_n$ with a vertex K_1 in common and it is symbolized by P_{n+1}^m This graph is presented in Figure 4. The Kulli path windmill graph P_3^m is a friendship graph. Let $P = P_{n+1}^m, m \geq 2, n \geq 5$. Then P has $mn+1$ vertices and $2mn - m$ edges. The graph P has four types of 2-distance degree of edges as given in Table 4.

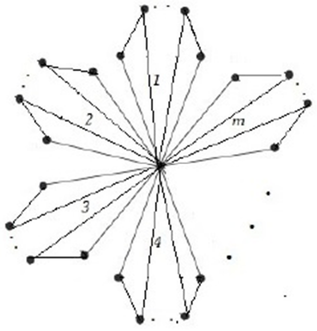

Figure 4: Kulli path windmill graph P_{n+1}^m.

Table 4: 2-distance degree edge partition of P

$d_2(u), d_2(v) \mid uv \in E(P)$	$(0, mn-2)$	$(0, mn-3)$	$(mn-2, mn-3)$	$(mn-3, mn-3)$
Number of edges	$2m$	$mn-2m$	$2m$	$mn-3m$

Theorem 5.1. *Let* $P = P_{n+1}^m, m \geq 2, n \geq 5$. *Then*

$$LM_1^*(P_{n+1}^m) \quad = \quad 3m^2n^2 - 2m^2n - 9mn + 10m.$$

Proof. By using Eq. (1.1) and Table 4, we obtain

$$\begin{aligned} LM_1^*(P_{n+1}^m) &= \sum_{uv\in E(P)} [d_2(u) + d_2(v)] \\ &= (0+mn-2)2m + (0+mn-3)(mn-2m) \\ &\quad +(mn-2+mn-3)2m \\ &\quad +(mn-3+mn-3)(mn-3m) \\ &= 3m^2n^2 - 2m^2n - 9mn + 10m. \end{aligned}$$

Theorem 5.2. *Let* $P_{n+1}^m, m \geq 2, n \geq 5$. *Then*

$$\begin{aligned} HLM_1(P_{n+1}^m) &= 5m^3n^3 - 4m^3n^2 - 30m^2n^2 + 36m^2n \\ &\quad + 45mn - 68m. \end{aligned}$$

Proof. From Eq. (1.2) and by using Table 4, we deduce

$$\begin{aligned} HLM_1(P_{n+1}^m) &= \sum_{uv\in E(P)} [d_2(u) + d_2(v)]^2 \\ &= (0+mn-2)^2 2m + (0+mn-3)^2(mn-2m) \\ &\quad +(mn-2+mn-3)^2 2m \\ &\quad +(mn-3+mn-3)^2(mn-3m) \\ &= 5m^3n^3 - 4m^3n^2 - 30m^2n^2 + 36m^2n + 45mn \\ &\quad -68m. \end{aligned}$$

Theorem 5.3. *Let* $P_{n+1}^m, m \geq 2, n \geq 5$. *Then*

$$\begin{aligned} HLM_2(P_{n+1}^m) &= (mn-3)^2(m^3n^2 + 2m^3n^2 - 6m^2n^2 \\ &\quad - 3m^3n + 10m^2n + 9mn - 19m). \end{aligned}$$

Proof. By using Eq. (1.3), we have

$$HLM_2(P_{n+1}^m) \quad = \quad \sum_{uv\in E(P)} [d_2(u)d_2(v)]^2$$

By using Table 4, we obtain

$$\begin{aligned} HLM_2(P_{n+1}^m) &= (0\times(mn-2))^2 2m + (0\times(mn-3))^2 \\ &\quad +[(mn-2)(mn-3)]^2 2m) \\ &\quad +[(mn-3)(mn-3)]^2(mn-3m \\ &= (mn-3)^2(m^3n^2 + 2m^3n^2 - 6m^2n^2 \\ &\quad -3m^3n + 10m^2n + 9mn - 19m). \end{aligned}$$

VII. CONCLUSION

In this paper, we have obtained the expressions for the first and second leap hyper-Zagreb indices of french windmill graphs, dutch windmill graphs, Kulli cycle windmill graphs and Kulli path windmill graphs.

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International Journal of Applied Engineering Research ISSN 0973-4562 Volume 14, Number 1 (2019) pp. 325 - 342
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Kulli-Basava Indices of Graphs

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ABSTRACT:
The mean isomer degeneracy d of a topological index decide its isomer discriminating power, the isomer discriminating power is high if $d = 1$ and the larger the d, the smaller is the isomer discriminating power. Bearing this in mind, we introduce new degree-based topological indices called Kulli-Basava indices and study their mathematical and chemical properties which have good response with the mean isomer degeneracy (i.e., the mean isomer degeneracy of modified first Kulli-Basava index is 1). Further, We obtain closed formulae for Kulli-Basava indices of some graph families and establish the relations connecting these new indices with other degree-based topological indices which are already in the literature. In addition, the Kulli-Basava indices of some graph operations are obtained.

AMS subject classification: 05C07, 05C76, 92E10.
Keywords: Kulli-Basava indices; graph operations; topological indices.

1. PRELIMINARIES

Let $G = (V, E)$ be a finite undirected graph with no loops and no multiple edges having V as its vertex set and E as its edge set. Let $|V| = n$ and $|E| = m$. A graph G is said to be r-regular if degree of each vertex in G is equal to r ($r \in Z^+$). The neighbourhood of a vertex $v \in V(G)$ is defined as the set $N_G(v)$ consisting of all vertices u which are adjacent to v in G. The degree of a vertex $v \in V(G)$, denoted by $d_G(v)$ and is defined as $|N_G(v)|$. The neighbourhood degree sum of a vertex $v \in V(G)$ is denoted by $S_G(v)$ and is defined as $S_G(v) = \sum\limits_{u\in N_G(v)} d_G(u)$. The *degree $d_G(e)$ of an edge $e = uv$* of G is given by $d_G(e) = d_G(u) + d_G(v) - 2$. We now define, an *edge neighbourhood of a vertex $v \in V(G)$* as the set $N_e(v)$ consisting of all edges e which are incident with v and the *edge neighbourhood degree sum of a vertex $v \in V(G)$* is denoted by $S_e(v)$ (If the graph is not specified then it can be denoted as $S_e(v/G)$) and is defined as $S_e(v) = \sum\limits_{e\in N_e(v)} d_G(e)$.

Topological indices are numerical values associated with the molecular graphs. In mathematical chemistry, these graph invariants are known as molecular descriptors. Topological indices play a vital role in mathematical chemistry specially, in chemical documentation, isomer discrimination, quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. *Wiener index* is the first topological index used by Wiener [30] in the year 1947, to calculate boiling point of paraffins. There after Gutman and Trinajstić defined *Zagreb indices* in 1972, which now are most popular and have many applications in chemistry. The following indices are useful for proving our results. The *first and second Zagreb indices* of a graph G are defined as follows [12]:

$$M_1(G) = \sum_{v\in V(G)} d_G(v)^2 and M_2(G) = \sum_{uv\in E(G)} d_G(u) \cdot d_G(v),$$

respectively. The *first Zagreb index* [23] can also be expressed as

$$M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)].$$

In [9], Fath-Tabar defined the *third Zagreb index* as

$$M_3(G) = \sum_{uv\in E(G)} |d_G(u) - d_G(v)|.$$

Another degree-based graph invariant,

$$F(G) = \sum_{v\in V(G)} d_G(v)^3 = \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2]$$

was encountered in [12]. This index is called "forgotten topological index"[10].
Later, it was Randić [27] who gave most chemically efficient topological index called *Randić index*, which is defined as

$$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_G(u) \cdot d_G(v)}}.$$

In [26], Shirdel et al. introduced a new version of Zagreb index named *hyper-Zagreb index* which is defined as

$$HM_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)]^2.$$

Further, in [31] Gao et al. defined the *second hyper Zagreb index* as

$$HM_2(G) = \sum_{uv\in E(G)} [d_G(u) \cdot d_G(v)]^2.$$

In [21], Li defined the *first general Zagreb index* as

$$M_1^{\alpha}(G) = \sum_{v\in V(G)} d_G(v)^{\alpha},$$

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where $\alpha \in Z^+$.

In [11], Graovac et al. defined *fifth M -Zagreb indices* as

$$M_1G_5(G) = \sum_{uv \in E(G)} [S_G(u) + S_G(v)]$$

$$\text{and } M_2G_5(G) = \sum_{uv \in E(G)} S_G(u) \cdot S_G(v). \tag{1.1}$$

In [18], Kulli defined the *fifth M_3-Zagreb index* as

$$M_3G_5(G) = \sum_{uv \in E(G)} |S_G(u) - S_G(v)|.$$

The *minus F-index* of a graph G is introduced by Kulli in [20], defined as

$$M_iF(G) = \sum_{uv \in E(G)} \left| d_G(u)^2 - d_G(v)^2 \right|$$

In [19], Kulli introduced the concept of *Gourava indices* and *coindices* of graphs. The *first* and *second Gourava indices* of a molecular graph G are defined as

$$GO_1(G) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + d_G(u) \cdot d_G(v)]$$

and

$$GO_2(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))(d_G(u) \cdot d_G(v)),$$

respectively. Recently in [5], Basavanagoud et al. defined a new topological index called the *first neighbourhood Zagreb index* as

$$NM_1(G) = \sum_{v \in V(G)} S_G(v)^2.$$

Since then the theory of topological indices has been developed into two broad categories namely, distance-based and degree-based topological indices. However, there are numerous degree-based topological indices which are found applicable and employed in QSPR/QSAR analysis. With this point of view, we now proceed to introduce new degree-based topological indices and would name them as *Kulli-Basava indices* which are defined as

$$\text{first Kulli-Basava index:} \quad KB_1(G) = \sum_{uv \in E(G)} \big(S_e(u) + S_e(v)\big), \tag{1.2}$$

$$\text{modified first Kulli-Basava index:} \quad KB_1^*(G) = \sum_{v \in V(G)} S_e(v)^2, \tag{1.3}$$

$$\text{second Kulli-Basava index:} \quad KB_2(G) = \sum_{uv \in E(G)} S_e(u) \cdot S_e(v), \tag{1.4}$$

$$\text{third Kulli-Basava index:} \quad KB_3(G) = \sum_{uv \in E(G)} \big(|S_e(u) - S_e(v)|\big). \tag{1.5}$$

The rest of the paper is organized as follows. In section 2, we obtain explicit formulae for Kulli-Basava indices of some graph families. In section 3, we study the chemical applicability of first Kulli-Basava index and modified first Kulli-Basava index. In section 4, we derive first Kulli-Basava and modified first Kulli-Basava indices of some graph operations.

2. KULLI-BASAVA INDICES OF SOME GRAPH FAMILIES

In this section, we obtain explicit formulae for *Kulli-Basava indices* of various graph families. We denote P_n, C_n, K_n, $K_{a,b}$, $K_{1,b}$ and W_n for a path, a cycle, a complete graph, a complete bipartite graph, a star and a wheel graph, respectively.

Lemma 2.1. *If G is any graph of order n and size m, then*

(i) $S_G(v) \geq d_G(v)$, *equality holds if and only if* $G = nK_1$ *or* $G = nK_2$.

(ii) $\sum_{v \in V(G)} S_G(v) \geq 2m$, *equality holds if and only if* $G = nK_1$ *or* $G = nK_2$.

(iii) $\sum_{v \in V(G)} S_G(v) = M_1(G)$.

(iv) $S_G(v) \leq \Delta(G) \cdot d_G(v)$, *equality holds if and only if G is regular.*

(v) $\sum_{v \in V(G)} S_G(v) \leq 2m\Delta(G)$, *equality holds if and only if G is regular.*

Lemma 2.2. *If G is any graph of order n and size m, then*

(i) $S_e(v) \geq 2d_G(v) - 2$, *equality holds if and only if G is regular.*

(ii) $\sum_{v \in V(G)} S_e(v) \geq 2(2m - n)$, *equality holds if and only if G is regular.*

(iii) $\sum_{v\in V(G)} S_e(v) = 2(M_1(G) - 2m)$.

(iv) $S_e(v) \leq 2\Delta(G)(d_G(v)-1)$, *equality holds if and only if G is regular.*

(v) $\sum_{v\in V(G)} S_e(v) \leq 2\Delta(G)(2m-n)$, *equality holds if and only if G is regular.*

Lemma 2.3. *If G is any graph of order n and size m, then*

$$S_e(v) = d_G(v)^2 - 2d_G(v) + S_G(v).$$

Proof. From the definition of $S_e(v)$ of a vertex $v \in V(G)$, we have

$$\begin{aligned} S_e(v) &= \sum_{e\in N_e(v)} d_G(e) \\ &= \sum_{u\in N_G(v)} (d_G(v) + d_G(u) - 2) \\ &= d_G(v)^2 + \sum_{u\in N_G(v)} d_G(u) - 2d_G(v) \\ &= d_G(v)^2 - 2d_G(v) + S_G(v). \end{aligned}$$

□

Theorem 2.4. *If G is an r-regular graph with n vertices, then*

$$\begin{aligned} KB_1(G) &= 4mr(r-1) = \frac{4m(r-1)M_1(G)}{nr}, \\ KB_1^*(G) &= 4nr^2(r-1)^2 = 4(r-1)^2M_1(G), \\ KB_2(G) &= 4mr^2(r-1)^2 = 4(r-1)^2M_2(G), \\ KB_3(G) &= 0 = M_3(G). \end{aligned}$$

Proof. If G is an r-regular graph with n vertices, then for any vertex $v \in V(G)$,

$$S_e(v) = 2r(r-1).$$

Therefore,

$$\begin{aligned} KB_1(G) &= \sum_{uv\in E(G)} \big(S_e(u) + S_e(v)\big) \\ &= \sum_{uv\in E(G)} 4r(r-1) \\ &= 4mr(r-1). \\ KB_1^*(G) &= \sum_{v\in V(G)} S_e(v)^2 \\ &= \sum_{v\in V(G)} (2r(r-1))^2 \\ &= 4nr^2(r-1)^2 \\ &= 4(r-1)^2M_1(G), \text{ as } M_1(G) = nr^2 \text{ for an } r\text{-regular graph.} \\ KB_2(G) &= \sum_{uv\in E(G)} S_e(u)\cdot S_e(v) \\ &= \sum_{uv\in E(G)} 4r^2(r-1)^2 \\ &= 4mr^2(r-1)^2 = 4(r-1)^2M_2(G), \text{ as } M_2(G) = mr^2 \text{ for an } r\text{-regular graph.} \\ KB_3(G) &= \sum_{uv\in E(G)} \big(|S_e(u) - S_e(v)|\big) \\ &= \sum_{uv\in E(G)} (0) \\ &= 0 = M_3(G), \text{ as } M_3(G) = 0, \text{ for an } r\text{-regular graph.} \end{aligned}$$

□

Corollary 2.5. *If C_n is a cycle of order n, then*

$$\begin{aligned} KB_1(C_n) &= 8n = 2M_1(C_n),\\ KB_1^*(C_n) &= 16n = 4M_1(C_n),\\ KB_2(C_n) &= 16n = 4M_2(C_n),\\ KB_3(C_n) &= 0 = M_3(C_n). \end{aligned}$$

Corollary 2.6. *If K_n is a complete graph of order n, then*

$$\begin{aligned} KB_1(K_n) &= 2n(n-1)^2(n-2) = 2(n-2)M_1(K_n),\\ KB_1^*(K_n) &= 4n(n-1)^2(n-2)^2 = 4(n-2)^2M_1(K_n),\\ KB_2(K_n) &= 2n(n-1)^3(n-2)^2 = 4(n-2)^2M_2(K_n),\\ KB_3(K_n) &= 0 = M_3(K_n). \end{aligned}$$

Theorem 2.7. *If P_n is a path with n vertices, then*

$$\begin{aligned} KB_1(P_n) &= \begin{cases} 0 & \text{if } n=2,\\ 2(4n-9) & \text{otherwise.} \end{cases}\\ KB_1^*(P_n) &= 4(4n-11) = M_1(P_n)+12n-38, \ \text{for } \ n\geq 4,\\ KB_2(P_n) &= \begin{cases} 0 & \text{if } n=2,\\ 4 & \text{if } n=3,\\ 15 & \text{if } n=4,\\ 2(8n-25) & \text{otherwise.} \end{cases}\\ KB_3(P_n) &= \begin{cases} 0 & \text{if } n=2,\\ 2 & \text{if } n=3,\\ 4 & \text{if } n=4,\\ 6 & \text{otherwise.} \end{cases} \end{aligned}$$

Proof. If P_n is a path with $n \geq 2$ vertices, then there are two pendant vertices with $S_e(v) = \begin{cases} 0 & \text{if } n=2,\\ 1 & \text{if otherwise,} \end{cases}$ and two vertices are with $S_e(v) = 3$, if $n \geq 4$ and the remaining $n-4$ vertices are with $S_e(v) = 4$. Therefore, by substituting these values in Eqs. (1.2), (1.3), (1.4) and (1.5), we get the desired results. ☐

Theorem 2.8. *If $K_{a,b}$ is a complete bipartite graph with $a+b$ vertices and ab edges for $1 \leq a \leq b$ where $a,b \in Z^+$, then*

$$\begin{aligned} KB_1(K_{a,b}) &= ab(a+b)(a+b-2) = (a+b-2)M_1(K_{a,b}),\\ KB_1^*(K_{a,b}) &= ab(a+b)(a+b-2)^2 = (a+b-2)^2M_1(K_{a,b}),\\ KB_2(K_{a,b}) &= a^2b^2(a+b-2)^2 = (a+b-2)^2M_2(K_{a,b}),\\ KB_3(K_{a,b}) &= ab(|a-b|)(a+b-2) = (a+b-2)M_3(K_{a,b}). \end{aligned}$$

Proof. Let $K_{a,b}$ be a complete bipartite graph with $a+b$ vertices. let $V(K_{a,b}) = V_1 \cup V_2$ where $|V_1| = a$ and $|V_2| = b$. For every vertex $v \in V(K_{a,b})$, $S_e(v) = \begin{cases} b(a+b-2) & \text{if } v \in V_1(K_{a,b}),\\ a(a+b-2) & \text{if } v \in V_2(K_{a,b}). \end{cases}$ If $uv \in E(K_{a,b})$, then either $u \in V_1$ and $v \in V_2$ or $v \in V_1$ and $u \in V_2$.

Therefore,

$$\begin{aligned} KB_1(K_{a,b}) &= \sum_{uv\in E(K_{a,b})} \big(S_e(u)+S_e(v)\big)\\ &= \sum_{uv\in E(K_{a,b})} (b(a+b-2)+a(a+b-2))\\ &= ab(a+b)(a+b-2). \end{aligned}$$

$$\begin{aligned}
KB_1^*(K_{a,b}) &= \sum_{v\in V(K_{a,b})} S_e(v)^2\\
&= \sum_{v\in V_1(K_{a,b})} (b(a+b-2))^2 + \sum_{v\in V_2(K_{a,b})} (a(a+b-2))^2\\
&= ab(a+b)(a+b-2)^2\\
&= (a+b-2)^2 M_1(K_{a,b}),\ \text{as } M_1(K_{a,b}) = ab(a+b).\\
KB_2(K_{a,b}) &= \sum_{uv\in E(K_{a,b})} S_e(u)\cdot S_e(v)\\
&= \sum_{uv\in E(K_{a,b})} (b(a+b-2))(a(a+b-2))\\
&= a^2b^2(a+b-2)^2 = (a+b-2)^2 M_2(G),\ \text{as } M_2(K_{a,b}) = a^2b^2.\\
KB_3(K_{a,b}) &= \sum_{uv\in E(K_{a,b})} \big(|S_e(u)-S_e(v)|\big)\\
&= \sum_{uv\in E(K_{a,b})} |b(a+b-2)-a(a+b-2)|\\
&= ab(|a-b|)(a+b-2) = (a+b-2)M_3(K_{a,b})\ \text{as } M_3(K_{a,b}) = ab(|a-b|).
\end{aligned}$$

□

Corollary 2.9. *If $K_{1,b}$ is a star graph with $b \geq 2$, then*

$$\begin{aligned}
KB_1(K_{1,b}) &= b(b^2-1),\\
KB_1^*(K_{1,b}) &= b(b+1)(b-1)^2,\\
KB_2(K_{1,b}) &= b^2(b-1)^2,\\
KB_3(K_{1,b}) &= b(b-1)^2.
\end{aligned}$$

Corollary 2.10. *If $K_{a,a}$ is a complete bipartite graph, then*

$$\begin{aligned}
KB_1(K_{a,a}) &= 4a^3(a-1),\\
KB_1^*(K_{a,a}) &= 8a^3(a-1)^2,\\
KB_2(K_{a,a}) &= 4a^4(a-1)^2,\\
KB_3(K_{a,a}) &= 0.
\end{aligned}$$

Theorem 2.11. *If W_n is a wheel graph with $n+1$ vertices and $2n$ edges, then*

$$\begin{aligned}
KB_1(W_n) &= n(n^2+4n+27),\\
KB_1^*(W_n) &= n(n+9)^2 + n^2(n+1)^2,\\
KB_2(W_n) &= n(n+9)(n^2+2n+9),\\
KB_3(W_n) &= n(|n^2-9|).
\end{aligned}$$

Proof. Let W_n be a wheel graph with $n+1$ vertices and $2n$ edges. For every vertex $v \in V(W_n)$, $S_e(v) = \begin{cases} n(n+1) & \text{if } v \text{ is a central vertex,}\\ n+9 & \text{otherwise.}\end{cases}$
Therefore, by substituting these values in Eqs. (1.2), (1.3), (1.4) and (1.5), we get the desired results. □

In the following theorem, Kulli-Basava indices are expressed in terms of other topological indices which are already in the literature.

Theorem 2.12. *If G is a graph with n vertices and m edges, then*

$$\begin{aligned}
KB_1(G) &= F(G) - 2M_1(G) + M_1G_5(G),\\
KB_1^*(G) &= M_1^4(G) + 4M_1(G) - 4F(G) + NM_1(G) - 8M_2(G) + 2GO_2(G),\\
KB_2(G) &= HM_2(G) + 4M_2(G) + M_2G_5(G) + M_1^4(G) - 2NM_1(G) - 2F(G) + 4GO_2(G),\\
KB_3(G) &\leq M_3G_5(G) - 2M_3(G) + M_iF(G).
\end{aligned}$$

Proof. By definition of first Kulli-Basava index, we have

$$\begin{aligned}
KB_1(G) &= \sum_{uv\in E(G)} (S_e(u)+S_e(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)^2-2d_G(u)+S_G(u)+d_G(v)^2-2d_G(v)+S_G(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)^2+d_G(v)^2)-2\sum_{uv\in E(G)} (d_G(u)+d_G(v))+\sum_{uv\in E(G)} (S_G(u)+S_G(v)) \\
&= F(G)-2M_1(G)+M_1G_5(G).
\end{aligned}$$

By definition of modified first Kulli-Basava index, we have

$$\begin{aligned}
KB_1^*(G) &= \sum_{v\in V(G)} S_e(v)^2 \\
&= \sum_{v\in V(G)} (d_G(v)^2-2d_G(v)+S_G(v))^2 \\
&= \sum_{v\in V(G)} d_G(v)^4+4\sum_{v\in V(G)} d_G(v)^2-4\sum_{v\in V(G)} d_G(v)^4+4\sum_{v\in V(G)} d_G(v)^3+\sum_{v\in V(G)} S_G(v)^2 \\
&\quad +2\sum_{v\in V(G)} d_G(v)^2S_G(v)-4\sum_{v\in V(G)} d_G(v)S_G(v) \\
&= M_1^4(G)+4M_1(G)-4F(G)+NM_1(G)-8M_2(G)+2GO_2(G).
\end{aligned}$$

By definition of second Kulli-Basava index, we have

$$\begin{aligned}
KB_2(G) &= \sum_{uv\in E(G)} (S_e(u)S_e(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)^2-2d_G(u)+S_G(u))(d_G(v)^2-2d_G(v)+S_G(v)) \\
&= \sum_{uv\in E(G)} (d_G(u)d_G(v))^2+4\sum_{uv\in E(G)} d_G(u)d_G(v)+\sum_{uv\in E(G)} S_G(v)S_G(u) \\
&\quad -2\sum_{uv\in E(G)} (d_G(u)S_G(v)+d_G(v)S_G(u))-2\sum_{uv\in E(G)} (d_G(u)^2d_G(v)+d_G(v)^2d_G(u)) \\
&\quad +\sum_{uv\in E(G)} (d_G(u)^2S_G(v)+d_G(v)^2S_G(u)) \\
&= HM_2(G)+4M_2(G)+M_2G_5(G)+M_1^4(G)-2NM_1(G)-2F(G)+4GO_2(G).
\end{aligned}$$

By definition of third Kulli-Basava index, we have

$$\begin{aligned}
KB_3(G) &= \sum_{uv\in E(G)} |S_e(u)-S_e(v)| \\
&= \sum_{uv\in E(G)} |d_G(u)^2-2d_G(u)+S_G(u)-d_G(v)^2+2d_G(v)-S_G(v)| \\
&\leq \sum_{uv\in E(G)} |d_G(u)^2-d_G(v)^2|-2\sum_{uv\in E(G)} |d_G(u)-d_G(v)|+\sum_{uv\in E(G)} |S_G(u)-S_G(v)| \\
&= M_iF(G)-2M_3(G)+M_3G_5(G).
\end{aligned}$$

□

3. ON CHEMICAL APPLICABILITY OF THE FIRST AND MODIFIED FIRST KULLI-BASAVA INDICES

The topological indices with the higher correlation factor are of foremost important in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. In this section, we discuss the linear regression analysis of first and modified first Kulli-Basava indices with entropy(S), acentric factor(AcentFac), enthalpy of vaporization (HVAP) and standard enthalpy of vaporization (DHVAP) of octane isomers on the degree-based topological indices of the corresponding molecular graph. The first and modified first Kulli-Basava indices were tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. The dataset of octane isomers(columns 1-5 of Table 2) are taken from above web link whereas last two column of Table 2 are computed by definition of first and modified first Kulli-Basava indices, respectively. Here, the correlation between acentric factor(AcentFac) and first Kulli-Basava index is **-0.97738** (See Fig. 1), between entropy and first Kulli-Basava index is **-0.95621** (See Fig. 2). Also, the correlation between acentric factor(AcentFac) and modified first Kulli-Basava index is **-0.96462** (See Fig. 5), between entropy and modified first Kulli-Basava index is **-0.94764** (See Fig. 6).

A major drawback of most of the topological indices is their degeneracy, i.e., two or more isomers posses the same topological index. But modified first Kulli-Basava index exceptional for octane isomers. Bonchev et al. [6] defined the mean isomer degeneracy as:

$$d = \frac{n}{t} \ ,$$

where n and t are the number of isomers considered and the number of distinct values that the index assumes for these isomers, respectively. Here, minimum value of d is 1. As the value of $'d'$ increases the isomer-discrimination power of the topological indices decreases. Thus, d can decide the discriminating power of an index. For octane isomers modified first Kulli-Basava index exhibits good response ($d = 1$).

Table 1: Mean isomer degeneracy (d) of different indices for octane isomers.

Index	**Mean isomer degeneracy (d)**
First Zagreb index (M_1)	3.000
Second Zagreb index (M_2)	1.286
Forgotten topological index (F)	2.571
Hosoya index (Z)	1.286
Connectivity index (χ)	1.125
Harary index (η)	1.059
First Kulli-Basava index (KB_1)	**1.125**
Modified first Kulli-Basava index (KB_1^*)	**1.000**

Table 2: Experimental values of the entropy, acentric factor, HVAP, DHVAP and the corresponding value of first and modified first Kulli-Basava indices of octane isomers.

Alkane	**S**	**AcentFac**	**DHVAP**	**HVAP**	KB_1	KB_1^*
n-octane	111.67	0.397898	9.915	73.19	46	84
2-methyl-heptane	109.84	0.377916	9.484	70.3	58	124
3-methyl-heptane	111.26	0.371002	9.521	71.3	60	136
4-methyl-heptane	109.32	0.371504	9.483	70.91	60	138
3-ethyl-hexane	109.43	0.362472	9.476	71.7	62	150
2,2-dimethyl-hexane	103.42	0.339426	8.915	67.7	88	258
2,3-dimethyl-hexane	108.02	0.348247	9.272	70.2	74	192
2,4-dimethyl-hexane	106.98	0.344223	9.029	68.5	72	178
2,5-dimethyl-hexane	105.72	0.35683	9.051	68.6	70	164
3,3-dimethyl-hexane	104.74	0.322596	8.973	68.5	92	286
3,4-dimethyl-hexane	106.59	0.340345	9.316	70.2	76	204
2-methyl-3-ethyl-pentane	106.06	0.332433	9.209	69.7	76	206
3-methyl-3-ethyl-pentane	101.48	0.306899	9.081	69.3	96	312
2,2,3-trimethyl-pentane	101.31	0.300816	8.826	67.3	106	344
2,2,4-trimethyl-pentane	104.09	0.30537	8.402	64.87	100	302
2,3,3-trimethyl-pentane	102.06	0.293177	8.897	68.1	105	341
2,3,4-trimethyl-pentane	102.39	0.317422	9.014	68.37	82	212
2,2,3,3-tetramethylbutane	93.06	0.255294	8.41	66.2	138	504

The linear regression models for the entropy, acentric factor, HVAP, and DHVAP using the data of Table 2 are obtained using the least squares fitting procedure as implemented in R software [28]. The fitted models for KB_1 are:

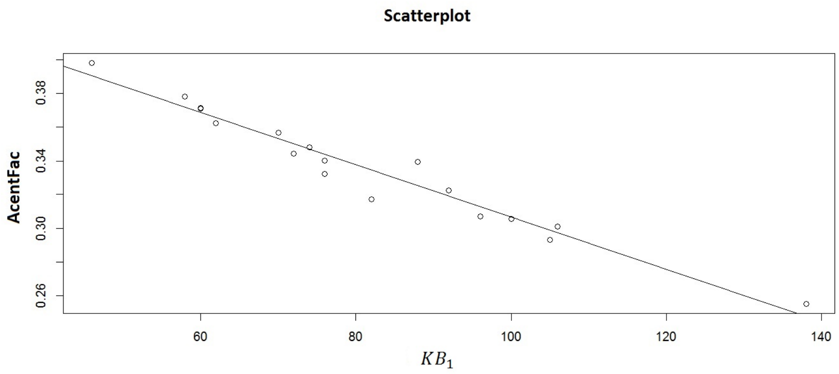


Figure 1: Scatter diagram of $AcentFac$ on KB_1 super imposed by the fitted regression line.

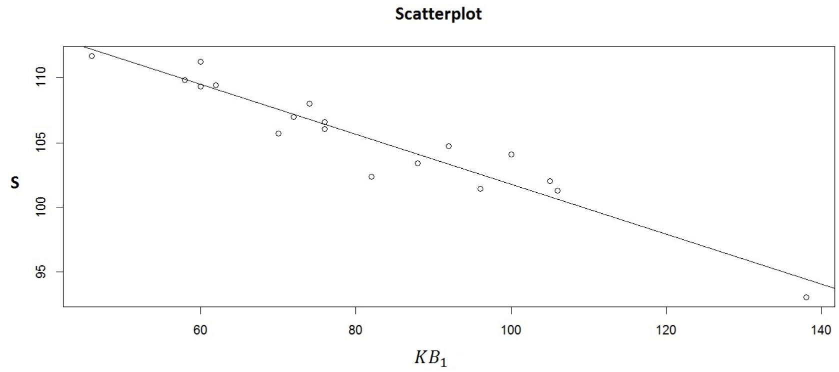


Figure 2: Scatter diagram of S on KB_1 super imposed by the fitted regression line.

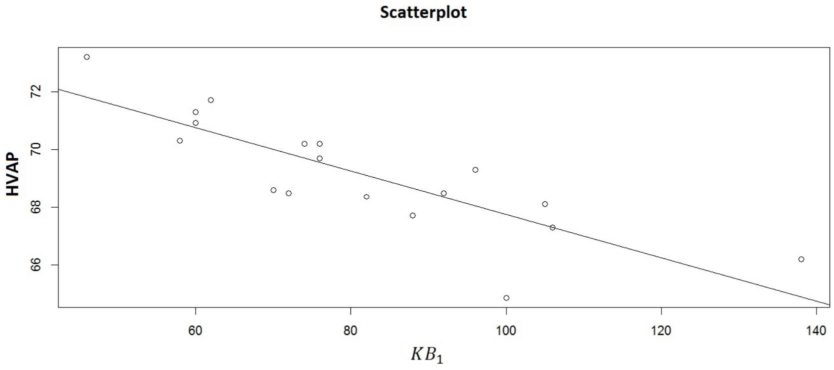


Figure 3: Scatter diagram of $HVAP$ on KB_1 super imposed by the fitted regression line.

$$\begin{aligned}
\widehat{AcentFac} &= 0.4615054(\pm 0.0070412) - 0.0015491(\pm 0.0000838)KB_1 && (3.1)\\
\hat{S} &= 121.08930(\pm 1.24186) - 0.19313(\pm 0.01478)KB_1 && (3.2)\\
\widehat{HVAP} &= 75.25859(\pm 1.06449) - 0.07510(\pm 0.01267)KB_1 && (3.3)\\
\widehat{DHVAP} &= 10.371745(\pm 0.160347) - 0.015344(\pm 0.001908)KB_1. && (3.4)
\end{aligned}$$

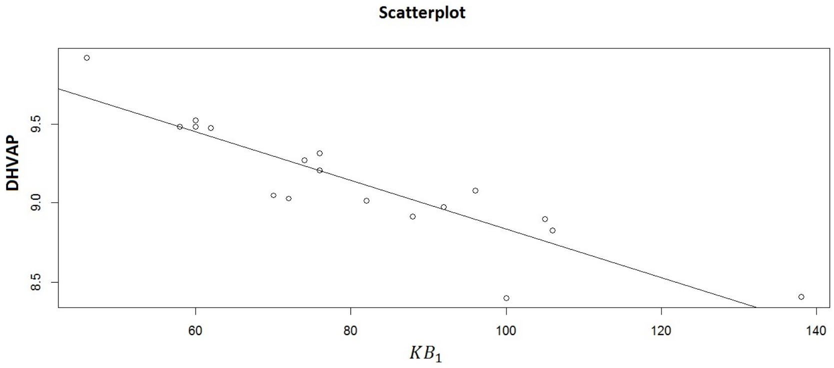


Figure 4: Scatter diagram of $DHVAP$ on KB_1 super imposed by the fitted regression line.

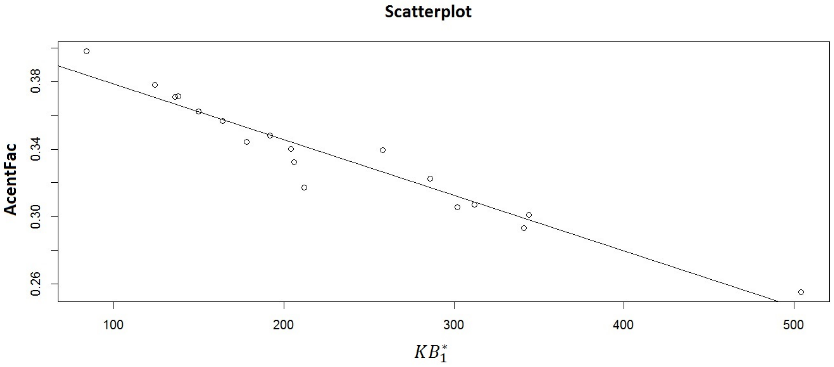


Figure 5: Scatter diagram of $AcentFac$ on KB_1^* super imposed by the fitted regression line.

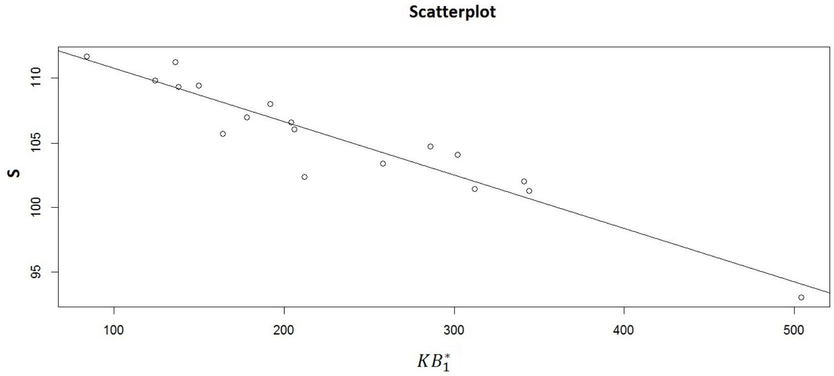


Figure 6: Scatter diagram of S on KB_1^* super imposed by the fitted regression line.

The fitted models for KB_1^* are:

$$\begin{aligned} Acen\hat{t}Fac &= 4.116e-01(\pm 5.655e-03) - 3.300e-04(\pm 2.255e-05)KB_1^* && (3.5)\\ \hat{S} &= 114.90369(\pm 0.87298) - 0.04131(\pm 0.00348)KB_1^* && (3.6)\\ HV\hat{A}P &= 72.667417(\pm 0.767163) - 0.015254(\pm 0.003059)KB_1^* && (3.7)\\ DH\hat{V}AP &= 9.8532852(\pm 0.1201055) - 0.0031645(\pm 0.0004788)KB_1^* && (3.8) \end{aligned}$$

Note: The values in brackets of the Eqs. (3.1) to (3.8) are the corresponding standard errors of the regression coefficients. The index is better as $|r|$ approaches 1. From Table 3, we can observe that KB_1 correlates highly with Acentric Factor and the correlation coefficient $|r| = 0.9773818$. Also KB_1 has good correlation ($|r| > 0.9$) with entropy, acentric factor and ($|r| > 0.8$) with HVAP, DHVAP. From Table 4, we can observe that KB_1^* correlates highly with Acentric Factor and the correlation coefficient

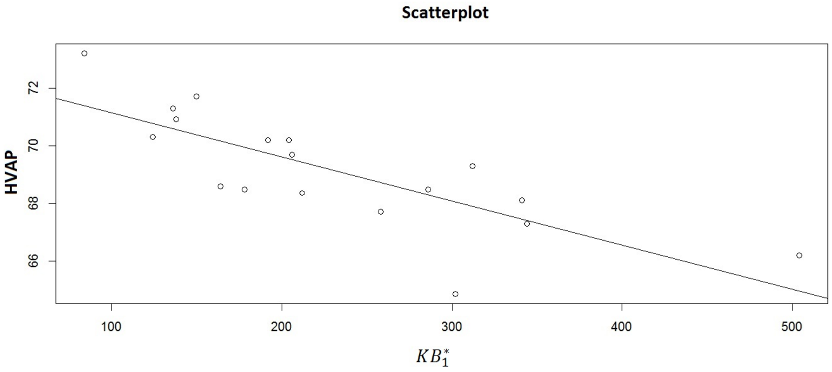


Figure 7: Scatter diagram of $HVAP$ on KB_1^* super imposed by the fitted regression line.

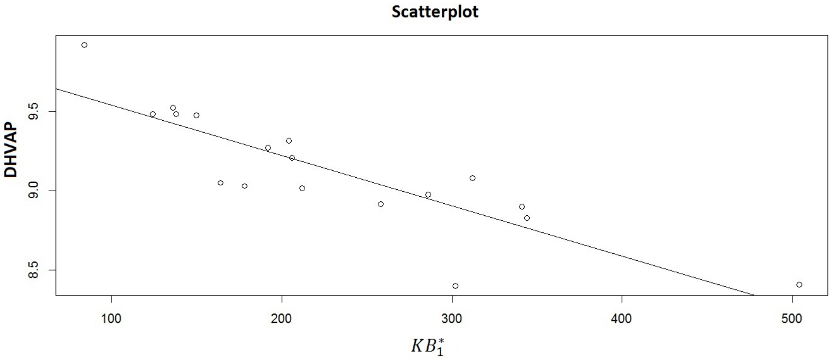


Figure 8: Scatter diagram of $DHVAP$ on KB_1^* super imposed by the fitted regression line.

Table 3: Correlation coefficient and residual standard error of regression models for KB_1

Physical Property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Acentric Factor	0.9773818	0.007728
Entropy	0.956207	1.363
HVAP	0.8289296	1.168
DHVAP	0.8953306	0.176

Table 4: Correlation coefficient and residual standard error of regression models for KB_1^*

Physical Property	Absolute value of the correlation coefficient ($\|r\|$)	Residual standard error
Acentric Factor	0.9646228	0.009633
Entropy	0.9476403	1.487
HVAP	0.7800876	1.307
DHVAP	0.8554989	0.2046

$|r| = 0.9646228$. Also KB_1^* has good correlation ($|r| > 0.9$) with entropy, acentric factor and ($|r| > 0.75$) with HVAP, DHVAP.

In the following section, we study the *first Kulli-Basava and modified first Kulli-Basava indices* of some graph operations such as cartesian product, composition, tensor product and corona of graphs, since the mean isomer degeneracy of these indices have good response.

4. FIRST KULLI-BASAVA AND MODIFIED FIRST KULLI-BASAVA INDICES OF SOME GRAPH OPERATIONS

Graph operations play an important role as some important graphs can be obtained by simple graph operations. For example, C_4-nanotorus, C_4-nanotube, planar grids, n-prism and Rook's graph are obtained by cartesian product of $C_m \times C_n$, $P_m \times C_n$, $P_n \times P_m$, $K_2 \times C_m$ and $K_n \times K_m$, respectively. Fence graph, closed fence graph and Catlin graph are obtained by composition of graphs. For more on graph operations we refer Imrich and Klavažar [15].

There are several papers devoted to topological indices of graph operations. To mention few, Khalifeh et al., obtained first and second Zagreb index of graph operations in [17], Aktaret al., obtained F-index in [1], Basavanagoud et al., obtained hyper-Zagreb index in [4, 3], N. De et al., obtained F-coindex in [7], Fath-Tabar derived GA_2 index in [8], Nadjafi-Arani et al., obtained degree distance based topological indices of tensor product of graphs in [22], Paulraj et al., computed degree distance of product graphs in [25], Yarahmadi et al., computed Szeged, vertex PI, first and second Zagreb indices of corona product of graphs in [32]. For some other topological indices of graph operations on can refer [16, 32] and references cited there in. At this stage, we evaluate *first Kulli-Basava and modified first Kulli-Basava indices* of some graph operations.

Definition 1. *The product [14] $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if and only if [$a = b$ and $xy \in E(H)$] or [$x = y$ and $ab \in E(G)$].*

Lemma 4.1. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$S_e((u,v)/G_1 \times G_2) = S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v)$$

Proof. By Lemma 2.3, we have

$$\begin{aligned} S_e((u,v)/G_1 \times G_2) &= d_{G_1\times G_2}(u,v)^2 - 2d_{G_1\times G_2}(u,v) + S_{G_1\times G_2}(u,v) \\ &= (d_{G_1}(u) + d_{G_2}(v))^2 - 2(d_{G_1}(u) + d_{G_2}(v)) + S_{G_1}(u) + S_{G_2}(v) + 2d_{G_1}(u)d_{G_2}(v) \\ &= S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v). \end{aligned}$$

□

Theorem 4.2. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1 \times G_2$ is given by*

$$KB_1(G_1 \times G_2) = (n_2 + 8m_2)KB_1(G_1) + (n_1 + 8m_1)KB_1(G_2) + 4(m_2M_1(G_1) + m_1M_1(G_2)) - 16m_1m_2.$$

Proof. By definition,

$$KB_1(G_1 \times G_2) = \sum_{(a,x)(b,y)\in E(G_1\times G_2)} (S_e((a,x)/G_1 \times G_2) + S_e((b,y)/G_1 \times G_2))$$

Using Lemma 4.1 we get,

$$\begin{aligned} &= \sum_{a\in V(G_1)} \sum_{xy\in E(G_2)} \big(S_e(a/G_1) + S_e(x/G_2) + 4d_{G_1}(a)d_{G_2}(x) + S_e(a/G_1) + S_e(y/G_2) + 4d_{G_1}(a)d_{G_2}(y)\big) \\ &\quad + \sum_{x\in V(G_2)} \sum_{ab\in E(G_1)} \big(S_e(x/G_2) + S_e(a/G_1) + 4d_{G_1}(a)d_{G_2}(x) + S_e(x/G_2) + S_e(b/G_1) + 4d_{G_1}(b)d_{G_2}(x)\big) \\ &= 4m_2(M_1(G_1) - 2m_1) + n_1KB_1(G_2) + 8m_1KB_1(G_2) + 4m_1(M_1(G_2) - 2m_2) + n_2KB_1(G_1) \\ &\quad +8m_2KB_1(G_1). \end{aligned}$$

□

Theorem 4.3. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1 \times G_2$ is given by*

$$\begin{aligned} KB_1^*(G_1 \times G_2) &= n_2KB_1^*(G_1) + n_1KB_1^*(G_2) + 8(M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + 16M_1(G_1)M_1(G_2) \\ &\quad +16m_2F(G_1) + 16m_1F(G_2) - 32m_2M_1(G_1) - 32m_1M_1(G_2) + 32m_2M_2(G_1) \\ &\quad +32m_1M_2(G_2). \end{aligned}$$

Proof. By definition, $KB_1^*(G_1 \times G_2) = \sum\limits_{(u,v)\in V(G_1\times G_2)} S_e((u,v)/G_1 \times G_2)^2$

Using Lemma 4.1 we get,

$$\begin{aligned}
&= \sum_{(u,v)\in V(G_1\times G_2)} \big(S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v)\big)^2 \\
&\quad + \sum_{u\in V(G_1)}\sum_{v\in V(G_2)} \big(S_e(u/G_1)^2 + S_e(v/G_2)^2 + 2S_e(u/G_1)S_e(v/G_2) + 16d_{G_1}(u)^2 d_{G_2}(v)^2 \\
&\quad +8(S_e(u/G_1) + S_e(v/G_2))d_{G_1}(u)d_{G_2}(v)\big) \\
&= n_2KB_1^*(G_1) + n_1KB_1^*(G_2) + 8(M_1(G_1) - 2m_1)(M_1(G_2) - 2m_2) + 16M_1(G_1)M_1(G_2) \\
&\quad +16m_2F(G_1) + 16m_1F(G_2) - 32m_2M_1(G_1) - 32m_1M_1(G_2) + 32m_2M_2(G_1) \\
&\quad +32m_1M_2(G_2).
\end{aligned}$$

□

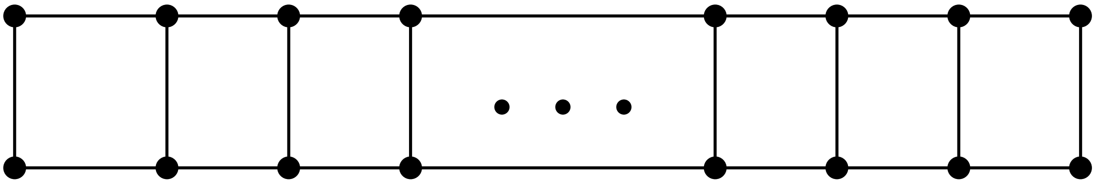


Figure 9: The Ladder graph L_n.

Corollary 4.4. *The ladder graph L_n is defined as the cartesian product of P_2 and P_n. From Theorem 4.3, we derive the following results.*

$$KB_1(L_n) = 4(22n - 49),$$
$$KB_1^*(L_n) = 8(36n - 71).$$

Corollary 4.5. *For a C_4-nanotorus, $TC_4(m,n) = C_m \times C_n$, the first Kulli-Basava and modified first Kulli-Basava indices are given by*

$$KB_1(TC_4(m,n)) = 160mn,$$
$$KB_1^*(TC_4(m,n)) = 576mn.$$

Corollary 4.6. *The cartesian product of P_n and C_m yields a C_4-nanotube, $TUC_4(m,n) = P_n \times C_m$. Its first Kulli-Basava and modified first Kulli-Basava indices are given by*

$$KB_1(TUC_4(m,n)) = 10m(16n - 25),$$
$$KB_1^*(TUC_4(m,n)) = 4m(144n - 227).$$

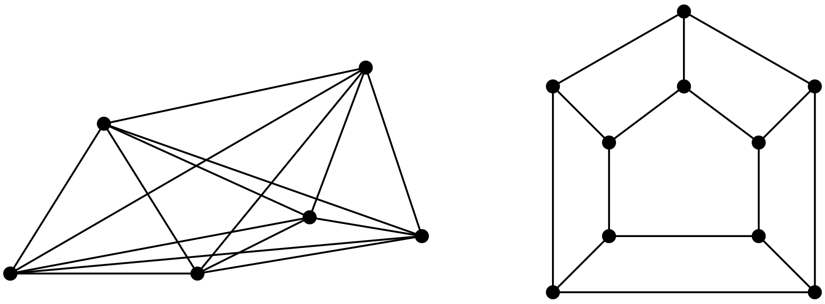
Corollary 4.7. *The first Kulli-Basava and modified first Kulli-Basava indices of planar grid $P_n \times P_m$ are given by*

$$KB_1(P_n \times P_m) = 2(88mn - 125m - 125n + 160),$$
$$KB_1^*(P_n \times P_m) = 4(144mn - 227m - 227n + 320).$$

Corollary 4.8. *For a n-prism, $K_2 \times C_n$, the first Kulli-Basava and modified first Kulli-Basava indices are given by*

$$KB_1(K_2 \times C_n) = 18n^2(n-1)^2(n-2) + 88n.$$
$$KB_1^*(K_2 \times C_n) = 288n.$$

Corollary 4.9. *The cartesian product of K_n and K_m yields the Rook's graph. Its first Kulli-Basava and modified first Kulli-Basava indices are given by*
$KB_1(K_n \times K_m) = 2mn((n-1)^2(n-2)(4m-3) + (m-1)^2(m-2)(4n-3))$
$+2mn(m-1)(n-1)(n+m-4)$.
$KB_1^*(K_n \times K_m) = 4mn((n-1)^2(n-2)^2 + (m-1)^2(m-2)^2)$
$+8mn(m-1)(n-1)(2m^2+2n^2+3mn-10m-10n+14)$.



$K_3 \times K_2$ $K_2 \times C_5$

Figure 10: The example of Rook's graph ($K_3 \times K_2$) and $n-$Prism graph ($n = 5$)

Definition 2. *The composition [14] $G[H]$ of graphs G and H with disjoint vertex sets $V(G)$ and $V(H)$ and edge sets $E(G)$ and $E(H)$ is the graph with vertex set $V(G[H]) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G[H]$ if and only if [a is adjacent to b] or [$a = b$ and x is adjacent to y].*

Lemma 4.10. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$\begin{aligned} S_e((u,v)/G_1[G_2]) &= n_2S_e(u/G_1) + S_e(v/G_2) + (n_2^2-n_2)(d_{G_1}(u)^2 + S_{G_1}(u)) + 2(m_2-n_2)d_{G_1}(u) \\ &\quad +3n_2d_{G_1}(u)d_{G_2}(v). \end{aligned}$$

Proof. By Lemma 2.3, we have

$$\begin{aligned} S_e((u,v)/G_1[G_2]) &= d_{G_1[G_2]}(u,v)^2 - 2d_{G_1[G_2]}(u,v) + S_{G_1[G_2]}(u,v) \\ &= (n_2d_{G_1}(u) + d_{G_2}(v))^2 - 2(d_{G_1}(u) + d_{G_2}(v)) + n_2^2S_{G_1}(u) + S_{G_2}(v) + 2m_2d_{G_1}(u) \\ &\quad +n_2d_{G_1}(u)d_{G_2}(v) \\ &= n_2S_e(u/G_1) + S_e(v/G_2) + (n_2^2-n_2)(d_{G_1}(u)^2 + S_{G_1}(u)) + 2(m_2-n_2)d_{G_1}(u) \\ &\quad +3n_2d_{G_1}(u)d_{G_2}(v). \end{aligned}$$

□

Theorem 4.11. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1[G_2]$ is given by*

$$\begin{aligned} KB_1(G_1[G_2]) &= n_2^3KB_1(G_1) + (n_1+6m_1n_2)KB_1(G_2) + n_2^3(n_2-n_1)F(G_1) + n_2^3(n_2-n_1)M_1G_5(G_1) \\ &\quad +2n_2(5m_2n_2 - n_2^2 + m_2)M_1(G_1) + 4m_1n_2M_1(G_2) + 4m_1m_2(n_2^2 - 7n_2 + 2m_2). \end{aligned}$$

Proof. By definition, $KB_1(G_1[G_2]) = \sum\limits_{(a,x)(b,y)\in E(G_1[G_2])} (S_e((a,x)/G_1[G_2]) + S_e((a,x)/G_1[G_2]))$

Using Lemma 4.10 we get,

$$\begin{aligned}
= &\sum_{x\in V(G_2)}\sum_{y\in V(G_2)}\sum_{ab\in E(G_1)}\big((n_2^2-n_2)(d_{G_1}(a)^2+S_{G_1}(a))+n_2S_e(a/G_1)+S_e(x/G_2)+2(m_2-n_2)d_{G_1}(a)\\
&+3n_2d_{G_1}(a)d_{G_2}(x)+(n_2^2-n_2)(d_{G_1}(b)^2+S_{G_1}(b))+n_2S_e(b/G_1)+S_e(y/G_2)+2(m_2-n_2)d_{G_1}(b)\\
&+3n_2d_{G_1}(b)d_{G_2}(y)\big)\\
&+\sum_{a\in V(G_1)}\sum_{xy\in E(G_2)}\big((n_2^2-n_2)(d_{G_1}(a)^2+S_{G_1}(a))+n_2S_e(a/G_1)+S_e(x/G_2)+2(m_2-n_2)d_{G_1}(a)\\
&+3n_2d_{G_1}(a)d_{G_2}(x)+(n_2^2-n_2)(d_{G_1}(a)^2+S_{G_1}(a))+n_2S_e(a/G_1)+S_e(y/G_2)+2(m_2-n_2)d_{G_1}(a)\\
&+3n_2d_{G_1}(a)d_{G_2}(y)\big).
\end{aligned}$$

Solving these summations one can get the desired result. ☐

Theorem 4.12. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1[G_2]$ is given by*

$$\begin{aligned}
KB_1^*(G_1[G_2]) = &\ n_2^2KB_1^*(G_1)+KB_1^*(G_2)+(n_2^4+n_2^3-2n_2^2)M_1^4(G_1)+(n_2^4+n_2^3-2n_2^2)NM_1(G_1)\\
&+2n_2^2(n_2^2-1)GO_2(G_1)+(28m_2^2n_2-64m_2n_2^2-16m_2n_2+4n_2^3+8n_2^2)M_1(G_1)\\
&+16m_1(m_2-2n_2)M_1(G_2)+(12m_2n_2^3+20m_2n_2^2-16n_2^3+8n_2^2)M_2(G_1)\\
&+24m_1n_2M_2(G_2)+n_2(13n_2+4)M_1(G_1)M_1(G_2)\\
&+(16m_2n_2^3-4m_2n_2^2+4m_2n_2-4n_2^4)F(G_1)+64m_1m_2n_2-32m_1m_2^2.
\end{aligned}$$

Proof. By definition, $KB_1^*(G_1[G_2])=\sum_{(u,v)\in V(G_1[G_2])}S_e((u,v)/G_1[G_2])^2$

Using Lemma 4.10 we get,

$$\begin{aligned}
= &\sum_{(u,v)\in V(G_1[G_2])}\big(n_2S_e(u/G_1)+S_e(v/G_2)+(n_2^2-n_2)(d_{G_1}(u)^2+S_{G_1}(u))+2(m_2-n_2)d_{G_1}(u)\\
&+3n_2d_{G_1}(u)d_{G_2}(v)\big)^2.
\end{aligned}$$

Solving this summation one can get the desired result. ☐

Definition 3. *The corona [14] $G_1\circ G_2$ of two graphs G_1 and G_2 of order n_1 and n_2 respectively, is defined as the graph obtained by taking one copy of G_1 and n_1 copies of G_2 and then joining the i^{th} vertex of G_1 to every vertex in the i^{th} copy of G_2.*

Lemma 4.13. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$S_e(v/G_1\circ G_2)=\begin{cases} S_e(v/G_1)+n_2^2+2n_2d_{G_1}(v)+2m_2 & \text{if } v\in V(G_1),\\ S_e(v/G_2)+3d_{G_2}(v)+d_{G_1}(v_i)+n_2-1 & \text{if } v\in V(G_2), v_i\in V(G_1).\end{cases}$$

Proof. By Lemma 2.3, we have $S_e(v/G_1\circ G_2)=d_{G_1\circ G_2}(v)^2-2d_{G_1\circ G_2}(v)+S_{G_1\circ G_2}(v)$

$$\begin{aligned}
&=\begin{cases}(d_{G_1}(v)+n_2)^2-2(d_{G_1}(v)+n_2)+S_{G_1}(v)+2(n_2+m_2) & \text{if } v\in V(G_1)\\ (d_{G_2}(v)+1)^2-2(d_{G_1}(v)+1)+S_{G_2}(v)+d_{G_2}(v)+d_{G_1}(v_i)+n_2 & \text{if } v\in V(G_2), v_i\in V(G_1)\end{cases}\\
&=\begin{cases}S_e(v/G_1)+n_2^2+2n_2d_{G_1}(v)+2m_2 & \text{if } v\in V(G_1)\\ S_e(v/G_2)+3d_{G_2}(v)+d_{G_1}(v_i)+n_2-1 & \text{if } v\in V(G_2), v_i\in V(G_1).\end{cases}
\end{aligned}$$

☐

Theorem 4.14. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1\circ G_2$ is given by*

$$\begin{aligned}
KB_1(G_1\circ G_2) = &\ KB_1(G_1)+n_1KB_1(G_2)+4n_2M_1(G_1)+5n_1M_1(G_2)\\
&+8m_1m_2+2m_1n_2(3n_2-1)+2n_1m_2(3n_2-1)+n_1n_2(n_2^2+n_2-1).
\end{aligned}$$

Proof. By definition, $KB_1(G_1 \circ G_2) = \sum\limits_{uv \in E(G_1 \circ G_2)} (S_e(u/G_1 \circ G_2) + S_e(v/G_1 \circ G_2))$

Using Lemma 4.13 we get,

$$\begin{aligned}
= & \sum_{uv \in E(G_1)} \big(S_e(u/G_1) + n_2^2 + 2n_2 d_{G_1}(u) + 2m_2 + S_e(v/G_1) + n_2^2 + 2n_2 d_{G_1}(v) + 2m_2\big) \\
& + \sum_{uv \in E(G_1)} \sum_{v_i \in V(G_1)} \big(S_e(u/G_2) + 3d_{G_2}(u) + d_{G_1(v_i)} + n_2 - 1 + S_e(v/G_2) + 3d_{G_2}(v) + d_{G_1(v_i)} + n_2 - 1\big) \\
& + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \big(S_e(u/G_1) + n_2^2 + 2n_2 d_{G_1}(u) + 2m_2 + S_e(v/G_2) + 3d_{G_2}(v) + d_{G_1}(u) + n_2 - 1\big).
\end{aligned}$$

Solving these summations one can get the desired result. □

Theorem 4.15. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1 \circ G_2$ is given by*

$$\begin{aligned}
KB_1^*(G_1 \circ G_2) &= KB_1^*(G_1) + n_1 KB_1^*(G_2) + (8n_2^2 - 7n_2 + 8m_2)M_1(G_1) + (9n_1 + 4n_2 + 8m_1 - 16)M_1(G_2) \\
&\quad + 4n_2 F(G_1) + 6F(G_2) + 8n_2 M_2(G_1) + 12M_2(G_2) + (n_1 + 8m_1 n_2)(n_2^2 + 2m_2)^2 \\
&\quad - 8m_1 n_2^2 + 8(3n_2 - 4)m_1 m_2 + n_1 n_2 (n_2 - 1)^2 + 8m_2(n_2 - 1).
\end{aligned}$$

Proof. By definition, $KB_1^*(G_1 \circ G_2) = \sum\limits_{v \in V(G_1 \circ G_2)} S_e(v/G_1 \circ G_2)^2$

Using Lemma 4.13 we get,

$$\begin{aligned}
= & \sum_{v \in V(G_1 \circ G_2)} \big(S_e(u/G_1) + S_e(v/G_2) + 4d_{G_1}(u)d_{G_2}(v)\big)^2 \\
= & \sum_{v \in V(G_1)} \big(S_e(v/G_1) + n_2^2 + 2n_2 d_{G_1}(v) + 2m_2\big)^2 \\
& + \sum_{u \in V(G_1)} \sum_{v \in V(G_2)} \big(S_e(v/G_2) + 3d_{G_2}(v) + d_{G_1}(u) + n_2 - 1\big)^2 \\
= & \; KB_1^*(G_1) + n_1 KB_1^*(G_2) + (8n_2^2 - 7n_2 + 8m_2)M_1(G_1) + (9n_1 + 4n_2 + 8m_1 - 16)M_1(G_2) \\
& + 4n_2 F(G_1) + 6F(G_2) + 8n_2 M_2(G_1) + 12M_2(G_2) + (n_1 + 8m_1 n_2)(n_2^2 + 2m_2)^2 \\
& - 8m_1 n_2^2 + 8(3n_2 - 4)m_1 m_2 + n_1 n_2 (n_2 - 1)^2 + 8m_2(n_2 - 1).
\end{aligned}$$

□

As an application of Theorem 4.14 and Theorem 4.15, we obtain explicit formulae for *first Kulli-Basava and modified first Kulli-Basava indices* of $k-$ thorny cycle $C_n \circ \overline{K_k}$.

Corollary 4.16. $KB_1(C_n \circ \overline{K_k}) = nk(k^2 + 7k + 13) + 8n$ *and*
$KB_1^*(C_n \circ \overline{K_k}) = n(8k^5 + k^4 + k^3 + 22k^2 + 37k + 16)$.

Definition 4. *The tensor product [29] $G_1 \circledast G_2$ of two graphs G_1 and G_2 of order n_1 and n_2 respectively, is defined as the graph with vertex set $V_1 \times V_2$ and (u_1, v_1) is adjacent with (u_2, v_2) if and only if $u_1 u_2 \in E(G_1)$ and $v_1 v_2 \in E(G_2)$.*

Lemma 4.17. *If G_1 and G_2 are two graphs of order n_1 and n_2 and size m_1 and m_2, respectively, then we have*

$$S_e((u,v)/G_1 \circledast G_2) = S_{G_1}(u)S_{G_2}(v) + d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v).$$

Proof. By Lemma 2.3, we have

$$\begin{aligned}
S_e((u,v)/G_1 \circledast G_2) &= d_{G_1 \circledast G_2}(u,v)^2 - 2d_{G_1 \circledast G_2}(u,v) + S_{G_1 \circledast G_2}(u,v) \\
&= d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v) + S_{G_1}(u)S_{G_2}(v).
\end{aligned}$$

□

Theorem 4.18. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then the first Kulli-Basava index of $G_1 \circledast G_2$ is given by*

$$KB_1(G_1 \circledast G_2) \quad = \quad F(G_1)F(G_2) - 2M_1(G_1)M_1(G_2) + NM_1(G_2)M_1G_5(G_1).$$

Proof. By definition,

$$KB_1(G_1 \circledast G_2) = \sum_{(a,x)(b,y)\in E(G_1\circledast G_2)} (S_e((a,x)/G_1 \circledast G_2) + S_e((b,y)/G_1 \circledast G_2))$$

Using Lemma 4.17 we get,

$$= \sum_{ab\in E(G_1)} \sum_{xy\in E(G_2)} \big(d_{G_1}(a)^2 d_{G_2}(x)^2 - 2d_{G_1}(a)d_{G_2}(x) + S_{G_1}(a)S_{G_2}(x)$$

$$+d_{G_1}(b)^2 d_{G_2}(y)^2 - 2d_{G_1}(b)d_{G_2}(y) + S_{G_1}(b)S_{G_2}(y)\big).$$

Solving these summations one can get the desired result. □

Theorem 4.19. *If G_1 and G_2 are two graphs of order n_1, n_2 and size m_1, m_2 respectively, then modified first Kulli-Basava index of $G_1 \circledast G_2$ is given by*

$$\begin{aligned} KB_1^*(G_1 \circledast G_2) \quad &= \quad M_1^4(G_1)M_1^4(G_2) + 4M_1(G_1)M_1(G_2) - 4F(G_1)F(G_2) + NM_1(G_1)NM_1(G_2) \\ &\quad +2GO_2(G_1)GO_2(G_2) - 16M_2(G_1)M_2(G_2). \end{aligned}$$

Proof. By definition, $KB_1^*(G_1 \circledast G_2) = \sum_{(u,v)\in V(G_1\circledast G_2)} S_e((u,v)/G_1 \circledast G_2)^2$

Using Lemma 4.17 we get,

$$\begin{aligned} &= \sum_{u\in V(G_1)} \sum_{v\in V(G_2)} \big(S_{G_1}(u)S_{G_2}(v) + d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v)\big)^2 \\ &= \sum_{u\in V(G_1)} \sum_{v\in V(G_2)} \big(S_{G_1}(u)^2 S_{G_2}(v)^2 + (d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v))^2 \\ &\quad +2S_{G_1}(u)S_{G_2}(v)(d_{G_1}(u)^2 d_{G_2}(v)^2 - 2d_{G_1}(u)d_{G_2}(v))\big) \\ &= M_1^4(G_1)M_1^4(G_2) + 4M_1(G_1)M_1(G_2) - 4F(G_1)F(G_2) + NM_1(G_1)NM_1(G_2) \\ &\quad +2GO_2(G_1)GO_2(G_2) - 16M_2(G_1)M_2(G_2). \end{aligned}$$

□

As an application of Theorem 4.18 and Theorem 4.19, we obtain following computations.

Corollary 4.20. *The first Kulli-Basava index of tensor product of different graphs is as follows:*
(i) $KB_1(P_n \circledast P_m) = 8(4n-7)(6m-13) - 8(2n-3)(2m-3), m, n \geq 3.$

(ii) $KB_1(P_n \circledast C_m) = 32m(5n-9), m, n \geq 3.$

(iii) $KB_1(P_n \circledast K_m) = 2m(m-1)^2(4m^2n - 7m^2 - 4mn + 7m - 4n + 6), m, n \geq 3.$

(iv) $KB_1(C_n \circledast C_m) = 160mn, m, n \geq 3.$

(v) $KB_1(C_n \circledast K_m) = 8mn(m-1)^2(m^2 - m - 1), m, n \geq 3.$

(vi) $KB_1(K_n \circledast K_m) = mn(m-1)^2(n-1)^2(2m^2 - 3m - n + mn + 1), m, n \geq 3.$

Corollary 4.21. *The modified first Kulli-Basava index of tensor product of different graphs is as follows:*
(i) $KB_1^*(P_n \circledast P_m) = 4(8m-15)(8n-15) + 16(2m-3)(2n-3) + 16(4m-7)(4n-7)$

$+ 4(8m - 19)(8n - 19) - 256(m - 2)(n - 2), m, n \geq 4.$

(ii) $KB_1^*(P_n \circledast C_m) = 32m(18n - 35), m \geq 3, n \geq 4.$

(iii) $KB_1^*(P_n \circledast K_m) = 4m(m - 1)^2(16m^2n - 31m^2 - 48mn + 92m + 36n - 67),$
$m \geq 3, n \geq 4.$

(iv) $KB_1^*(C_n \circledast C_m) = 576mn, m, n \geq 3.$

(v) $KB_1^*(C_n \circledast K_m) = 16mn(m - 1)^2(4m^2 - 12m + 9), m, n \geq 3.$

(vi) $KB_1^*(K_n \circledast K_m) = 4mn(m - 1)^4(n - 1)^4 + 4mn(m - 1)^2(n - 1)^2$
$- 8mn(m - 1)^3(n - 1)^3, m, n \geq 3.$

Similarly, one can find the expressions for the second and third Kulli-Basava indices of these graph operations.

5. CONCLUSION

In this paper, we proposed a set of new topological indices called Kulli-Basava indices. We have explicitly studied first Kulli-Basava and modified first Kulli-Basava indices of some graph families. Further, we have obtained first Kulli-Basava and modified first Kulli-Basava indices of some graph operations. In addition, we have studied the chemical applicability of these indices. In future, one can derive the results for some other graph operations.

Acknowledgement
This work is partially supported by the University Grants Commission (UGC), Government of India, New Delhi, through UGC-SAP-DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I).
This work is supported by Directorate of Minorities, Government of Karnataka, Bangalore, through M. Phil/Ph. D Fellowship - 2017-18: No. DOM/FELLOWSHIP/CR-29/2017-18 dated: 09th Aug. 2017.

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Original Research Paper

Volume-9 | Issue-8 | August - 2019 | PRINT ISSN No. 2249 - 555X

Statistics

A STUDY OF SOCIO-ECONOMIC STATUS OF WORKING WOMEN BASED ON ECONOMIC FACTOR MONTHLY SAVINGS OF THE THREE DISTRICTS OF THE STATE KARNATAKA - A CASE STUDY

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ABSTRACT Women constitute the backbone of any nation. Prosperity of the nation depends upon the prosperity of its women. The financial demands of the Indian families are becoming rise day by day, working women in the contemporary society are also increasing day by day particularly in the urban area mainly due to the impact of education, employment opportunities, women reservation policies, self employment, and so on to mention a few. This paper is mainly analyze the socio-economic status of working women of the three districts of Karnataka state based on different demographic factors age, education, marital status, family type, with their monthly saving. Chi-square test is used to test the association between different demographic factors and monthly savings using SPSS 20 package.

KEYWORDS : Chi-Square test, Socio-economic , Monthly savings, Demographic Factors.

1. INTRODUCTION

Globalization ,liberalization and privatization are increased the opportunities in active participation of any economic activities irrespective of gender in particular women work force. The percentage of women in the active work population has increased rapidly in many countries around the world, including in India. The investigation of women participation in various types of occupation in the rural and urban area of three districts viz: Belgaum, Vijaypur and Bagalkot of Karnataka state is dealt by Hungund. C.P.S. and Vinayak. S Kulkarani (3).In this paper an association between demographic factor and their monthly savings of working women were identified using chi-square test. In this paper the socio-economic status of working women basing on different demographic factors with respect to their monthly savings was done through collecting primary data using questionnaire method, observations and interviews by 500 respondents. The collected data has been classified and obtained a frequency and percentage distribution basing on demographic factors and monthly savings. The association between various demographic factors and monthly savings were tested by using chi-square test and also measured the strength of the association between them using SPSS package.

2. Review of Literature

Shaik Ali (2014)[1] in his paper stated that compare to urban working women with rural working women their socio- economic status is low because ,among the 200 respondents in their survey 64 % of women were depends on agricultural based work and live in rural area and 36 % were other occupations live in urban area. The rural area working women get very low wages than urban working women, due to lack opportunities in workforce in rural area than the urban. Hence they conclude that if the monthly income a person's is low than it affects the socioeconomic status of their family and future.

Menon (1973)[2] in his study found that "The family or a person with having good income defiantly his socio-economic status is high than a person with having low income groups, it affects on academic achievements of their children's in school is better performance ".

3. Data Sources and Methods

Primary data was collected through questionnaire, observation and interviews. The univariate and bivariate data analysis was presented for the descriptive statistical data, which is the simple and best way to present numeric percentage. The chi-square test is used to test the association between socio-economic status based on their monthly savings and demographic factors age , education , marital status and family type. Among the total 500 samples 330 (66%) working women belongs to urban area and 170 (34 %) are from rural area. The district wise statistical analysis reveals that 54% of working women are from Bagalakot, 26% are from Vijayapur and 20% of working women belongs to Belagavi.

4. Preliminary Analysis of Classified Data

The classified data of respondents basing on different types of occupations by area is presented and analyzed in the paper C.P.S. Hungund and V.S. Kulkarani(1). The distribution of types of occupations of 500 respondents with respect to area is presented in the following table.

Table 4.1 : Distribution of respondents by types of occupation and area

Sl. No.	Types of occupation	Rural	Urban	Total
1	Bank/ Co-operative societies/LIC	15 (30%)	35 (70%)	50 (100%)
2.	Anganawadi staff/ supervisor	15 (30%)	35 (70%)	50 (100%)
3.	Catering/ mess/ Cooking/warden	10 (25%)	30 (75%)	40 (100%)
4.	College teachers	15 (30%)	35 (70%)	50 (100%)
5.	Doctors/ Nurse/ medical staff	15 (25%)	45 (75%)	60 (100%)
6.	Daily wages/ others	25 (50%)	25 (50%)	50 (100%)
7.	Owen Business handling/Entrepreneurs	15 (37.5%)	25 (62.5%)	40 (100%)
8	Government / Non-Government office staff	15 (30%)	35 (70%)	50 (100%)
9.	School Teachers	25 (42%)	35 (58%)	60 (100%)
10.	Tailoring and Garments	20 (40%)	30 (60%)	50 (100%)
	Total (N)	170 (34%)	330(66%)	500 (100%)

*(**Source:*** Primary *Survey)*

From the table 4.1 it could be seen that among the 170 rural respondents 25 are ST and DW each followed by 20 respondents TG and 15 of each respondents belongs to occupations type BLC, CDP, CT, EO, GNS etc. In urban area among the total 330 respondents 45 are belonging to occupations type DNMS , followed by occupations type BLC, CDP , CT , GNS ST are 35 respondents in each.

Table 4.2 : Distribution of respondents by demographic characteristics

Demographic characters	No. of respondents (%)	Demographic characters	No. of respondents (%)
Age (yr)		**Education**	
20 - 35	129 (26 %)	Primary/ SSLC	169 (34 %)
35 – 50	256 (51.2%)	PUC/ Degree	260 (52%)
50 & above	115 (23%)	P.G / Ph.D	71 (14.2%)
Marital Status		**Family type**	
Un - married	115 (23 %)	Single	370 (74%)
Married	385 (67%)	Joint	130 (26%)
Total	**500**	**Total**	**500**

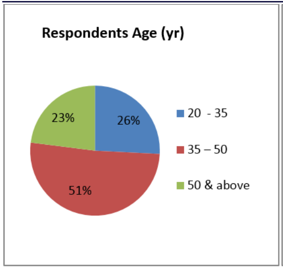

Figure -1

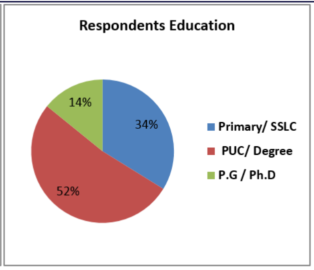

Figure – 2

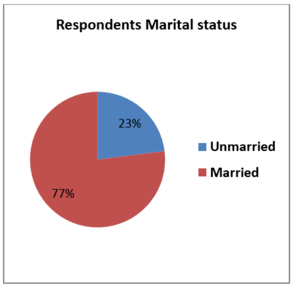

Figure -3

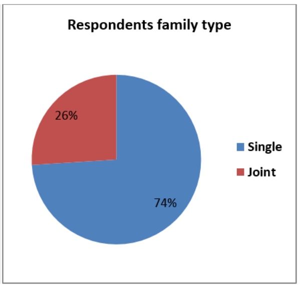

Figure – 4

4 : Association between demographic factors and socio- economic status based on monthly savings of the respondents.

In this section, where association between different demographic factors and monthly savings were identified using chi-square test.

4.1 Association between age and monthly savings

H0: There is no significant association between age and monthly savings.

Table 4.1 :Age and monthly savings of the respondents.

Age (yr)		Monthly savings (%)			Total
		Below 10	10 – 20	Above 20	
20 – 35	Count	35	54	40	129
	% within Age	27.1%	41.9%	31.0%	100.0%
35 – 50	Count	87	145	24	256
	% within Age	34.0%	56.6%	9.4%	100.0%
Above 50	Count	40	45	30	115
	% within Age	34.8%	39.1%	26.1%	100.0%
Total	Count	162	244	94	500
	% within Age	32.4%	48.8%	18.8%	100.0%

Table 4.1(a) :Chi-square test for age and monthly savings of the respondents

	Value	df	Asymp. Sig. (2-sided)
Pearson Chi-Square	33.776^{a}	4	.0001
Likelihood Ratio	34.617	4	.0001
Linear-by-Linear Association	2.372	1	.124
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 21.62.			

From the above table we conclude that, the result is significant since significant value is less than 0.05. Hence we reject null hypothesis. Which indicates that there is an association between demographic factor age and monthly savings.

Table 4.1(b) Symmetric Measures of age of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.260	.0001
	Cramer's V	.184	.0001
	Contingency Coefficient	.252	.0001
	N of Valid Cases	500	

From the above table symmetric measures reveals that the strength of the association between demographic factor age and monthly savings is 0.184. Which indicates 18.4 % of association between age and monthly savings.

4.2 Association between education and monthly savings

H0: There is no significant association between education and monthly savings.

Table 4.2 : Education and monthly savings of the respondents.

Education		Monthly savings(%)			Total
		Low	medium	High	
Primary/ SSLC	Count	67	89	13	169
	% within Education	39.6%	52.7%	7.7%	100.0%
PUC /Degree	Count	75	122	63	260
	% within Education	28.8%	46.9%	24.2%	100.0%
P.G/Ph.D	Count	20	33	18	71
	% within Education	28.2%	46.5%	25.4%	100.0%
Total	Count	162	244	94	500
	% within Education	32.4%	48.8%	18.8%	100.0%

Table 4.2(a) :Chi-square test for education monthly savings of the respondents

	Value	Df	Asymp. Sig. (2-sided)
Pearson Chi-Square	21.718a	4	.0001
Likelihood Ratio	24.295	4	.0001
Linear-by-Linear Association	13.698	1	.0001
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 13.35.			

From the above table it revealed that, the result is significant since significant value is less than 0.05. Hence we reject null hypothesis. which indicates that there is an association between demographic factor education and monthly savings.

Table 4.2(b) :Symmetric Measures education of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.208	.0001
	Cramer's V	.147	.0001
	Contingency Coefficient	.204	.0001
	N of Valid Cases	500	

From the above table symmetric measures reveals that the strength of the association between demographic factor education and monthly savings is 0.147. Which indicates 14.7 % of association between education and monthly savings.

4.3 Association between marital status and monthly savings

H0: There is no significant association between marital status and monthly savings.

Table 4.3 : Marital status and monthly savings of the respondents.

Marital Status		Monthly Savings (%)			Total
		Below 10	10 - 20	Above 20	
Un -Married	Count	26	51	38	115
	% within row	22.6%	44.3%	33.0%	100.0%
married	Count	136	193	56	385
	% within row	35.3%	50.1%	14.5%	100.0%
Total	Count	162	244	94	500
	% within row	32.4%	48.8%	18.8%	100.0%

Table 4.3(a) :Chi-square test for marital status and monthly savings of the respondents

	Value	Df	Asymp. Sig. (2-sided)
Pearson Chi-Square	21.143^{a}	2	.0001
Likelihood Ratio	19.541	2	.0001
Linear-by-Linear Association	17.447	1	.0001
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 21.62.			

From the above table it is clear that, the result is significant since significant value is less than 0.05. Hence we reject null hypothesis, which indicates that there is an association between demographic factor marital status and monthly savings.

Table 4.3(b) : symmetric Measures of marital status of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.206	.0001
	Cramer's V	.206	.0001

	Contingency Coefficient	.201	.0001
	N of Valid Cases	500	

The symmetric measures reveals that the strength of the association between demographic factor marital status and monthly savings is 0.206. Which indicates 20.6 % of association between marital status and monthly savings.

4.4 Association between family type and monthly savings

H0: There is no significant association between family type and monthly savings.

Table 4.4 : Family type and monthly savings of the respondents.

		Monthly Savings (%)			Total
Family type		Below 10	10 - 20	Above 20	
Single	Count	124	183	63	370
	% within row	33.5%	49.5%	17.0%	100.0%
Joint	Count	38	61	31	130
	% within row	29.2%	46.9%	23.8%	100.0%
Total	Count	162	244	94	500
	% within row	32.4%	48.8%	18.8%	100.0%

Table 4.4(a) :Chi-square test for family type and monthly savings of the respondents

	Value	Df	Asymp. Sig. (2-sided)
Pearson Chi-Square	3.051a	2	.218
Likelihood Ratio	2.945	2	.229
Linear-by-Linear Association	2.398	1	.122
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 24.44.			

From the above table it revealed that, the result is not significant since significant value is more than 0.05. Hence we accept null hypothesis, which indicates that there is no association between demographic factor family type and monthly savings.

Table 4.4 (b) : Symmetric measures family type of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.078	.218
	Cramer's V	.078	.218
	Contingency Coefficient	.078	.218
	N of Valid Cases	500	

From the above table symmetric measures reveals that the strength of the association between demographic factor family type and monthly savings is 0.078. Which indicates 7.8 % of weak association between family type and monthly savings.

5.CONCLUSION

The active participation of women in educational ,political ,social and economic activities in the nation refers to women empowerment. The socio - economic status of women is the base for women empowerment and prosperity of the nation, the socio-economic status of women uplift their position in the society. When the data were analyzed we have seen there is an association between the demographic factor age, education and type of family with socio-economic factor monthly savings and its percentage of association shows 18 ,15 and 21 respectively. If the monthly income of working women is good, than their monthly savings is also good ,the monthly savings is not for their individual it is for the whole family and children's future. The research findings reveals that the demographic factors age, education and family type are influence the socio- economic status of working women mainly on their monthly income and savings.

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Original Research Paper

Volume-9 | Issue-8 | August - 2019 | PRINT ISSN No. 2249 - 555X

Statistics

A STUDY OF SOCIO-ECONOMIC STATUS OF WORKING WOMEN BASED ON ECONOMIC FACTOR MONTHLY SAVINGS OF THE THREE DISTRICTS OF THE STATE KARNATAKA - A CASE STUDY

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ABSTRACT Women constitute the backbone of any nation. Prosperity of the nation depends upon the prosperity of its women. The financial demands of the Indian families are becoming rise day by day, working women in the contemporary society are also increasing day by day particularly in the urban area mainly due to the impact of education, employment opportunities, women reservation policies, self employment, and so on to mention a few. This paper is mainly analyze the socio-economic status of working women of the three districts of Karnataka state based on different demographic factors age, education, marital status, family type, with their monthly saving. Chi-square test is used to test the association between different demographic factors and monthly savings using SPSS 20 package.

KEYWORDS : Chi-Square test, Socio-economic , Monthly savings, Demographic Factors.

1. INTRODUCTION

Globalization ,liberalization and privatization are increased the opportunities in active participation of any economic activities irrespective of gender in particular women work force. The percentage of women in the active work population has increased rapidly in many countries around the world, including in India. The investigation of women participation in various types of occupation in the rural and urban area of three districts viz: Belgaum, Vijaypur and Bagalkot of Karnataka state is dealt by Hungund. C.P.S. and Vinayak. S Kulkarani (3).In this paper an association between demographic factor and their monthly savings of working women were identified using chi-square test. In this paper the socio-economic status of working women basing on different demographic factors with respect to their monthly savings was done through collecting primary data using questionnaire method, observations and interviews by 500 respondents. The collected data has been classified and obtained a frequency and percentage distribution basing on demographic factors and monthly savings. The association between various demographic factors and monthly savings were tested by using chi-square test and also measured the strength of the association between them using SPSS package.

2. Review of Literature

Shaik Ali (2014)[1] in his paper stated that compare to urban working women with rural working women their socio- economic status is low because ,among the 200 respondents in their survey 64 % of women were depends on agricultural based work and live in rural area and 36 % were other occupations live in urban area. The rural area working women get very low wages than urban working women, due to lack opportunities in workforce in rural area than the urban. Hence they conclude that if the monthly income a person's is low than it affects the socioeconomic status of their family and future.

Menon (1973)[2] in his study found that "The family or a person with having good income defiantly his socio-economic status is high than a person with having low income groups, it affects on academic achievements of their children's in school is better performance ".

3. Data Sources and Methods

Primary data was collected through questionnaire, observation and interviews. The univariate and bivariate data analysis was presented for the descriptive statistical data, which is the simple and best way to present numeric percentage. The chi-square test is used to test the association between socio-economic status based on their monthly savings and demographic factors age , education , marital status and family type. Among the total 500 samples 330 (66%) working women belongs to urban area and 170 (34 %) are from rural area. The district wise statistical analysis reveals that 54% of working women are from Bagalakot, 26% are from Vijayapur and 20% of working women belongs to Belagavi.

4. Preliminary Analysis of Classified Data

The classified data of respondents basing on different types of occupations by area is presented and analyzed in the paper C.P.S. Hungund and V.S. Kulkarani(1). The distribution of types of occupations of 500 respondents with respect to area is presented in the following table.

Table 4.1 : Distribution of respondents by types of occupation and area

Sl. No.	Types of occupation	Rural	Urban	Total
1	Bank/ Co-operative societies/LIC	15 (30%)	35 (70%)	50 (100%)
2.	Anganawadi staff/ supervisor	15 (30%)	35 (70%)	50 (100%)
3.	Catering/ mess/ Cooking/warden	10 (25%)	30 (75%)	40 (100%)
4.	College teachers	15 (30%)	35 (70%)	50 (100%)
5.	Doctors/ Nurse/ medical staff	15 (25%)	45 (75%)	60 (100%)
6.	Daily wages/ others	25 (50%)	25 (50%)	50 (100%)
7.	Owen Business handling/Entrepreneurs	15 (37.5%)	25 (62.5%)	40 (100%)
8	Government / Non-Government office staff	15 (30%)	35 (70%)	50 (100%)
9.	School Teachers	25 (42%)	35 (58%)	60 (100%)
10.	Tailoring and Garments	20 (40%)	30 (60%)	50 (100%)
	Total (N)	170 (34%)	330(66%)	500 (100%)

*(**Source:** Primary Survey)*

From the table 4.1 it could be seen that among the 170 rural respondents 25 are ST and DW each followed by 20 respondents TG and 15 of each respondents belongs to occupations type BLC, CDP, CT, EO, GNS etc. In urban area among the total 330 respondents 45 are belonging to occupations type DNMS , followed by occupations type BLC, CDP , CT , GNS ST are 35 respondents in each.

Table 4.2 : Distribution of respondents by demographic characteristics

Demographic characters	No. of respondents (%)	Demographic characters	No. of respondents (%)
Age (yr)		**Education**	
20 - 35	129 (26 %)	Primary/ SSLC	169 (34 %)
35 – 50	256 (51.2%)	PUC/ Degree	260 (52%)
50 & above	115 (23%)	P.G / Ph.D	71 (14.2%)
Marital Status		**Family type**	
Un - married	115 (23 %)	Single	370 (74%)
Married	385 (67%)	Joint	130 (26%)
Total	**500**	**Total**	**500**

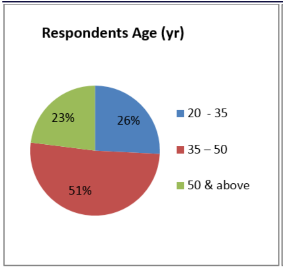

Figure -1

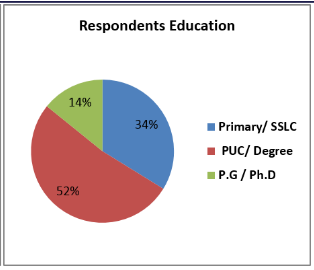

Figure – 2

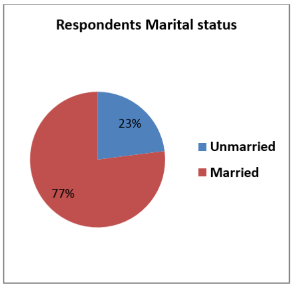

Figure -3

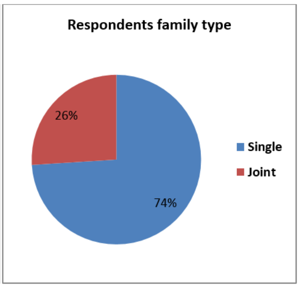

Figure – 4

4 : Association between demographic factors and socio- economic status based on monthly savings of the respondents.

In this section, where association between different demographic factors and monthly savings were identified using chi-square test.

4.1 Association between age and monthly savings

H0: There is no significant association between age and monthly savings.

Table 4.1 :Age and monthly savings of the respondents.

Age (yr)		Monthly savings (%)			Total
		Below 10	10 – 20	Above 20	
20 – 35	Count	35	54	40	129
	% within Age	27.1%	41.9%	31.0%	100.0%
35 – 50	Count	87	145	24	256
	% within Age	34.0%	56.6%	9.4%	100.0%
Above 50	Count	40	45	30	115
	% within Age	34.8%	39.1%	26.1%	100.0%
Total	Count	162	244	94	500
	% within Age	32.4%	48.8%	18.8%	100.0%

Table 4.1(a) :Chi-square test for age and monthly savings of the respondents

	Value	df	Asymp. Sig. (2-sided)
Pearson Chi-Square	33.776[a]	4	.0001
Likelihood Ratio	34.617	4	.0001
Linear-by-Linear Association	2.372	1	.124
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 21.62.			

From the above table we conclude that, the result is significant since significant value is less than 0.05. Hence we reject null hypothesis. Which indicates that there is an association between demographic factor age and monthly savings.

Table 4.1(b) Symmetric Measures of age of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.260	.0001
	Cramer's V	.184	.0001
	Contingency Coefficient	.252	.0001
	N of Valid Cases	500	

From the above table symmetric measures reveals that the strength of the association between demographic factor age and monthly savings is 0.184. Which indicates 18.4 % of association between age and monthly savings.

4.2 Association between education and monthly savings

H0: There is no significant association between education and monthly savings.

Table 4.2 : Education and monthly savings of the respondents.

Education		Monthly savings(%)			Total
		Low	medium	High	
Primary/ SSLC	Count	67	89	13	169
	% within Education	39.6%	52.7%	7.7%	100.0%
PUC /Degree	Count	75	122	63	260
	% within Education	28.8%	46.9%	24.2%	100.0%
P.G/Ph.D	Count	20	33	18	71
	% within Education	28.2%	46.5%	25.4%	100.0%
Total	Count	162	244	94	500
	% within Education	32.4%	48.8%	18.8%	100.0%

Table 4.2(a) :Chi-square test for education monthly savings of the respondents

	Value	Df	Asymp. Sig. (2-sided)
Pearson Chi-Square	21.718a	4	.0001
Likelihood Ratio	24.295	4	.0001
Linear-by-Linear Association	13.698	1	.0001
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 13.35.			

From the above table it revealed that, the result is significant since significant value is less than 0.05. Hence we reject null hypothesis. which indicates that there is an association between demographic factor education and monthly savings.

Table 4.2(b) :Symmetric Measures education of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.208	.0001
	Cramer's V	.147	.0001
	Contingency Coefficient	.204	.0001
	N of Valid Cases	500	

From the above table symmetric measures reveals that the strength of the association between demographic factor education and monthly savings is 0.147. Which indicates 14.7 % of association between education and monthly savings.

4.3 Association between marital status and monthly savings

H0: There is no significant association between marital status and monthly savings.

Table 4.3 : Marital status and monthly savings of the respondents.

Marital Status		Monthly Savings (%)			Total
		Below 10	10 - 20	Above 20	
Un -Married	Count	26	51	38	115
	% within row	22.6%	44.3%	33.0%	100.0%
married	Count	136	193	56	385
	% within row	35.3%	50.1%	14.5%	100.0%
Total	Count	162	244	94	500
	% within row	32.4%	48.8%	18.8%	100.0%

Table 4.3(a) :Chi-square test for marital status and monthly savings of the respondents

	Value	Df	Asymp. Sig. (2-sided)
Pearson Chi-Square	21.143[a]	2	.0001
Likelihood Ratio	19.541	2	.0001
Linear-by-Linear Association	17.447	1	.0001
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 21.62.			

From the above table it is clear that, the result is significant since significant value is less than 0.05. Hence we reject null hypothesis, which indicates that there is an association between demographic factor marital status and monthly savings.

Table 4.3(b) : symmetric Measures of marital status of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.206	.0001
	Cramer's V	.206	.0001

	Contingency Coefficient	.201	.0001
	N of Valid Cases	500	

The symmetric measures reveals that the strength of the association between demographic factor marital status and monthly savings is 0.206. Which indicates 20.6 % of association between marital status and monthly savings.

4.4 Association between family type and monthly savings

H0: There is no significant association between family type and monthly savings.

Table 4.4 : Family type and monthly savings of the respondents.

		Monthly Savings (%)			Total
Family type		Below 10	10 - 20	Above 20	
Single	Count	124	183	63	370
	% within row	33.5%	49.5%	17.0%	100.0%
Joint	Count	38	61	31	130
	% within row	29.2%	46.9%	23.8%	100.0%
Total	Count	162	244	94	500
	% within row	32.4%	48.8%	18.8%	100.0%

Table 4.4(a) :Chi-square test for family type and monthly savings of the respondents

	Value	Df	Asymp. Sig. (2-sided)
Pearson Chi-Square	3.051a	2	.218
Likelihood Ratio	2.945	2	.229
Linear-by-Linear Association	2.398	1	.122
N of Valid Cases	500		
a. 0 cells (.0%) have expected count less than 5. The minimum expected count is 24.44.			

From the above table it revealed that, the result is not significant since significant value is more than 0.05. Hence we accept null hypothesis, which indicates that there is no association between demographic factor family type and monthly savings.

Table 4.4 (b) : Symmetric measures family type of the respondents

		Value	Approx. Sig.
Nominal by Nominal	Phi	.078	.218
	Cramer's V	.078	.218
	Contingency Coefficient	.078	.218
	N of Valid Cases	500	

From the above table symmetric measures reveals that the strength of the association between demographic factor family type and monthly savings is 0.078. Which indicates 7.8 % of weak association between family type and monthly savings.

5.CONCLUSION

The active participation of women in educational ,political ,social and economic activities in the nation refers to women empowerment. The socio - economic status of women is the base for women empowerment and prosperity of the nation, the socio-economic status of women uplift their position in the society. When the data were analyzed we have seen there is an association between the demographic factor age, education and type of family with socio-economic factor monthly savings and its percentage of association shows 18 ,15 and 21 respectively. If the monthly income of working women is good, than their monthly savings is also good ,the monthly savings is not for their individual it is for the whole family and children's future. The research findings reveals that the demographic factors age, education and family type are influence the socio- economic status of working women mainly on their monthly income and savings.

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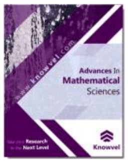

Original Research Article

ON THE INVARIANT OF NEW DEGREE-BASED TOPOLOGICAL INDICES OF SILICATE CHAIN GRAPH

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ABSTRACT

Throughout this paper simple and undirected graphs are considered. Let G = (V, E) be such a graph. The structure of a chemical compound can be represented by a graph whose vertex and edge specify the atom and bonds respectively. In this paper we compute certain topological indices of silicate chain.

Keywords: Chemical graph, topological indices, silicate chain graph

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PUBLICATION HISTORY

Received: May 31, 2019
Accepted: June 13, 2019

ARTICLE ID: AMS-74

1. INTRODUCTION

In chemical graph theory, we have many different topological index of arbitrary molecular graph *G*. A topological index of a graphs is a member related to a graph which is invariant under graph automorphisms, obviously, every topological index defines a counting polynomial and vice versa [1, 2].

Construction of the Silicate Chain Graph:

SiO_4 tetrahedral are found nearly in all the silicates. Silicates are immensely essential and complicated minerals. We get silicate from metal carbonates with sand or from fusing metal oxides. Silicates behave as the building blocks of the usual rock-forming minerals [3]. Consider a single tetrahedron (i.e., a pyramid having a triangular base). Place oxygen atoms at the four corners of a tetrahedron, and the silicon atom is bonded with equally-spaced atoms of oxygen. The resulting tetrahedron is a silicate tetrahedron, which is shown in figure 1a, and when this tetrahedron join with other tetrahedral joins with other tetrahedral linearly, then a single-row silicate chain is formed, as shown in figure 1b. When two tetrahedral join together corner-to-corner, then each tetrahedron shares its oxygen atom with the other tetrahedron, as shown in figure 1c. After this sharing, these two tetrahedral can be joined with two other tetrahedral, as in figure 1e, were *m* is the number of row lines and *n* is the number of edges in a row line [3].

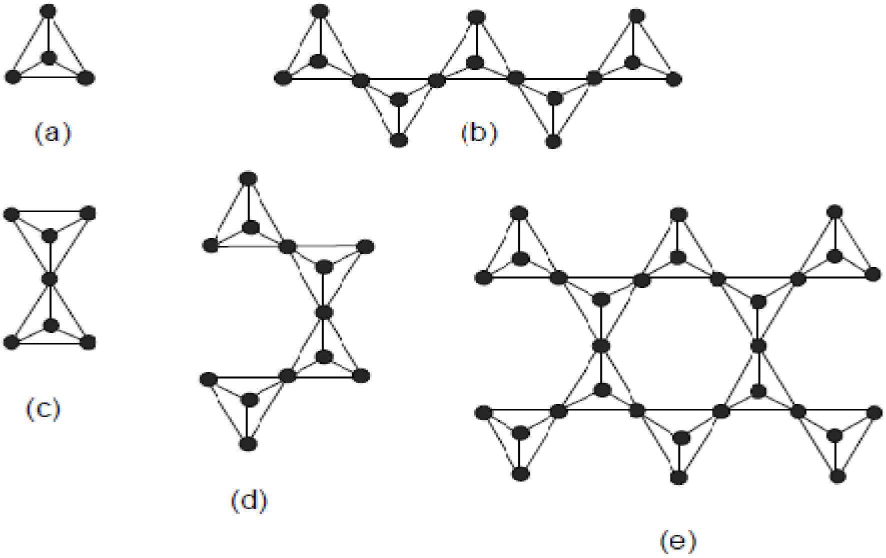

Figure 1. Chain silicate network

2. Survey of Certain Degree-Based Topological Indices

Motivated by previous research on Nanotubes [3-9], here we compute the values of two new topological indices of silicate chain.

***SK_3* Index:** The SK_3 index of a graph $G = (V, E)$ is defined as,

$$SK_3(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2} \qquad (1)$$

Where, $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbors of vertex u (or v) in G.

$S_G(u) = \sum_{u,v\in E(G)} d_G(u)$ and $N_G(u) = \{v\in V(G)/uv\in E(G)\}$

Arithmetic-Geometric (*AG_2*) Index: Let $G = (V, E)$ be a molecular graph, and $S_G(u)$ is the degree of the vertex u, then AG_2 index of G is defined as

$$AG_2(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u).S_G(v)}} \qquad (2)$$

Where, $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbors of vertex u (or v) in G.

$S_G(u) = \sum_{u,v\in E(G)} d_G(u)$ and $N_G(u) = \{v\in V(G)/uv\in E(G)\}$

3. RESULTS AND DISCUSSION

In this section, we calculate the closed results for topological indices, which based on vertex degrees of the m^{th} silicate chain. We compute the. The number of edges of the m^{th} chain silicate are 6mn. In the following theorem, the degree-based topological indices for the m^{th} chain silicate is computed.

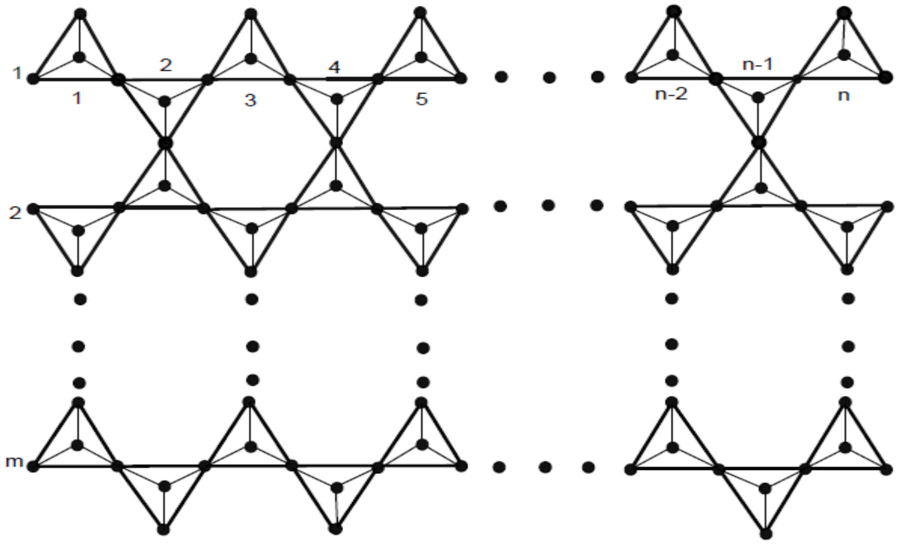

Figure 2. *mth* chain silicate *(SL(m,n))*

Table 1: Edge partition of silicate chain (SL(m,n)) when m<n and m is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-7
(15,15)	3m-3	(18,24)	2
(15,24)	2m+2n+2	(18,27)	m+3n-11
(12,24)	6	(18,30)	3mn-6m-7n+16
(15,27)	m+7n-23	(24,30)	2
(24,27)	m+n-1	(27,30)	m+5n-17
(24,24)	2	(30,30)	3mn-4m-12n+26

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$$SK_3\,(G) = 162mn - 55m - 79.5n + 52.5$$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 1 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv \in E(G)} \frac{S_G(u) + S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)[12] + (3m-3)[15] + (2m+2n+2)[19.5] + (6)[18] + (m+7n-23)[21] +$$

$$(m+n-1)[25.5] + (2)[24] + (m+n-7)[27] + (2)[21] + (m+3n-11)[22.5] +$$

$$(3mn-6m-7n+16)[24] + (2)[27] + (m+5n-17)[28.5] + (3mn-4m-12n+26)[30]$$

$$= 162mn - 55m - 79.5n + 52.5.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2(G) = 6.096mn + 0.8015m + 0.614n - 7.1893$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 1 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (3m-3) + (2m+2n+2)[1.027] + (6)[1.060] + (m+7n-23)[1.043] + (m+n-1)[1.0017) + 2 +$$

$$(m+n-7) + (2)[1.010] + (m+3n-11)[1.02] + (3mn-6m-7n+16)[1.032] + (2)[1.0062] +$$

$$(m+5n-17)[1.0013] + (3mn-4m-12n+26)$$

$$= 6.096mn + 0.8015m + 0.614n - 7.1893.$$

Table 2. Edge partition of silicate chain (SL(m,n)) when m<n and m is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	12	(27,27)	m+n-7
(15,15)	3m-6	(18,24)	4
(15,24)	m+3n-11	(18,27)	m+3n-11
(12,24)	12	(18,30)	3mn-5m-8n+18
(15,27)	m+7n-23	(24,30)	4
(24,27)	m+n-1	(27,30)	m+5n-17
(24,24)	0	(30,30)	3mn-4m-12n+26

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3(G) = 162mn - 51m - 84n + 216$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 2 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$
$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$
$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$
$$= (12)[12] + (3m-6)[15] + (m+3n-11)[19.5] + (12)[18] + (m+7n-23)[21] +$$
$$(m+n-1)[25.5] + (0)[24] + (m+n-7)[27] + (4)[21] + (m+3n-11)[22.5] +$$
$$(3mn-5m-8n+18)[24] + (4)[27] + (m+5n-17)[28.5] + (3mn-4m-12n+26)[30]$$

$$= 162mn - 51m - 84n + 216.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2(G) = 6.096mn - 0.067m - 0.1942n + 0.0542$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 2 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 12 + (3m-6) + (m+3n-11)[1.027] + (12)[1.060] + (m+7n-23)[1.043] + (m+n-1)[1.0017) +$$

$$(m+n-7) + (4)[1.010] + (m+3n-1)[1.02] + (3mn-5m-8n+18)[1.032] + (4)[1.0062] +$$

$$(m+5n-17)[1.0013] + (3mn-4m-12n+26)$$

$$= 6.096mn - 0.067m - 0.1942n + 0.0542.$$

Table 3. Edge partition of silicate chain (SL(m,n)) when m<n, m and n is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-6
(15,15)	3m-2	(18,24)	2
(15,24)	m+3n-2	(18,27)	4m-6
(12,24)	6	(18,30)	3mn+3m-16n+36
(15,27)	2m+6n-24	(24,30)	2
(24,27)	m+n-2	(27,30)	m+5n-20
(24,24)	2	(30,30)	3mn-16m+8

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

SK₃ (G) $= 162mn - 211.5m - 4.5n - 27$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 3 we can apply the formula of *SK₃* index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$
\begin{aligned}
&= (6)\left[12\right] + (3m-2)[15] + (m+3n-2)[19.5] + (6)[18] + (2m+6n-24)[21] + \\
&(m+n-2)[25.5] + (2)[24] + (m+n-6)[27] + (2)[21] + (4m-6)[22.5] + \\
&(3mn+3m-16n+36)[24] + (2)[27] + (m+5n-20)[28.5] + (3mn-16m+8)[30]
\end{aligned}
$$

$$= 162mn - 211.5m - 4.5n - 27\,.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2\ (G)\ = 6.096mn + 0.29m - 01648n + 0.309$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 3 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$
\begin{aligned}
&= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] + \\
&(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] + \\
&(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] + \\
&(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right] \\
&= 6 + (3m-2) + (m+3n-2)[1.027] + (6)[1.060] + (2m+6n-24)[1.043] + (m+n-2)[1.0017) + \\
&(2) + (m+n-6)[1] + (2)[1.010] + (4m-6)[1.02] + (3mn+3m-16n+36)[1.032] + (2)[1.0062] + \\
&(m+5n-20)[1.0013] + (3mn-16m+8) \\
&= 6.096mn + 0.29m - 01648n + 0.309\,.
\end{aligned}
$$

Table 4. Edge partition of silicate chain (SL(m,n)) when m<n , m and n is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-6
(15,15)	3m-2	(18,24)	2
(15,24)	m+3n-2	(18,27)	m+3n-12
(12,24)	6	(18,30)	3mn-13m+4
(15,27)	m+7n-26	(24,30)	2
(24,27)	m+n-2	(27,30)	m+5n-20
(24,24)	2	(30,30)	3mn+4m-20n+48

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3\ (G)\ = 162mn - 3m - 132n + 192$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 4 we can apply the formula of *SK₃* index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv \in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)\left[12\right] + (3m-2)[15] + (m+3n-2)[19.5] + (6)[18] + (m+7n-26)[21] +$$

$$(m+n-2)[25.5] + (2)[24] + (m+n-6)[27] + (2)[21] + (m+3n-12)[22.5] +$$

$$(3mn-13m+4)[24] + (2)[27] + (m+5n-20)[28.5] + (3mn+4m-20n+48)[30]$$

$$= 162mn - 3m - 132n + 192.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

AG₂ (G) $= 6.096mn - 0.323m + 0.4502n + 1.079$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 4 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv \in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (3m-2) + (m+3n-2)[1.027] + (6)[1.060] + (m+7n-26)[1.043] + (m+n-2)[1.0017) +$$

$$(2) + (m+n-6)[1] + (2)[1.010] + (m+3n-12)[1.02] + (3mn-13m+4)[1.032] + (2)[1.0062] +$$

$$(m+5n-20)[1.0013] + (3mn+4m-20n+48)$$

$$= 6.096mn - 0.323m + 0.4502n + 1.079.$$

Table 5. Edge partition of silicate chain (SL(m,n)) when m>n m is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-9
(15,15)	m+2n-3	(18,24)	2
(15,24)	m+3n+7	(18,27)	m+3n-9
(12,24)	6	(18,30)	3mn-5m-8n+11
(15,27)	m+7n-17	(24,30)	2
(24,27)	m+n+1	(27,30)	m+5n-11
(24, 24)	2	(30,30)	3mn-2m-14n+12

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$$SK_3(G) = 162mn - 21m - 181.5n - 29$$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 5 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)[12] + (m+2n-3)[15] + (m+3n-2)[19.5] + (6)[18] + (m+7n-17)[21] +$$

$$(m+n+1)[25.5] + (2)[24] + (m+n-9)[27] + (2)[21] + (m+3n-9)[22.5] +$$

$$(3mn-5m-8n+1)[24] + (2)[27] + (m+5n-11)[28.5] + (3mn-2m-14n+12)[30]$$

$$= 162mn - 21m - 181.5n - 29.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$$AG_2(G) = 6.096mn - 0.067m + 0.1942n + 9.8 * 10^{-03}$$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 5 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n))

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (m+2n-3) + (m+3n+7)[1.027] + (6)[1.060] + (m+7n-17)[1.043] + (m+n+1)[1.0017) +$$

$$(2) + (m+n-9)[1] + (2)[1.010] + (m+3n-9)[1.02] + (3mn-5m-8n+1)[1.032] + (2)[1.0062] +$$

$$(m+5n-11)[1.0013] + (3mn-2m-14n+12)$$

$$= 6.096mn - 0.067m + 0.1942n + 9.8*10^{-03}$$

Table 6. Edge partition of silicate chain (SL(m,n)) when m>n and m is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	12	(27,27)	m+n-9
(15,15)	m+2n-6	(18,24)	4
(15,24)	m+3n-5	(18,27)	m+3n-9
(12,24)	12	(18,30)	3mn-5m-8n+12
(15,27)	m+7n-17	(24,30)	4
(24,27)	m+n+1	(27,30)	m+5n-11
(24,24)	0	(30,30)	3mn-2m-14n+12

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

SK_3 *(G)* $= 162mn - 21m + 264n + 29.5$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 6 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G)=\sum_{uv\in E(G)}\frac{S_G(u)+S_G(v)}{2}$$

$$=(12,12)\left[\frac{12+12}{2}\right]+(15,15)\left[\frac{15+15}{2}\right]+(15,24)\left[\frac{15+24}{2}\right]+(12,24)\left[\frac{12+24}{2}\right]+(15,27)\left[\frac{15+27}{2}\right]+$$

$$(24,27)\left[\frac{24+27}{2}\right]+(24,24)\left[\frac{24+24}{2}\right]+(27,27)\left[\frac{27+27}{2}\right]+(18,24)\left[\frac{18+24}{2}\right]+(18,27)\left[\frac{18+27}{2}\right]+$$

$$(18,30)\left[\frac{18+30}{2}\right]+(24,30)\left[\frac{24+30}{2}\right]+(27,30)\left[\frac{27+30}{2}\right]+(30,30)\left[\frac{30+30}{2}\right]$$

$$=(6)[12]+(m+2n-6)[15]+(m+3n-5)[19.5]+(12)[18]+(m+7n-17)[21]+$$

$$(m+n+1)[25.5]+(0)[24]+(m+n-9)[27]+(4)[21]+(m+3n-9)[22.5]+$$

$$(3mn-5m-8n+12)[24]+(4)[27]+(m+5n-11)[28.5]+(3mn-2m-14n+12)[30]$$

$$=162mn-21m+264n+29.5.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2(G)=6.096mn-0.067m+0.1942n+0.3334$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 6 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G)=\sum_{uv\in E(G)}\frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$=(12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right]+(15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right]+(15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right]+(12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right]+$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right]+(24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right]+(24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right]+(27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right]+$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right]+(18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right]+(18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right]+(24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right]+$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right]+(30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$=21+(m+2n-6)+(m+3n-5)[1.027]+(12)[1.060]+(m+7n-17)[1.043]+(m+n+1)[1.0017)+$$

$$(0)+(m+n-9)[1]+(4)[1.010]+(m+3n-9)[1.02]+(3mn-5m-8n+12)[1.032]+(4)[1.0062]+$$

$$(m+5n-11)[1.0013]+(3mn-2m-14n+12)$$

$$=6.096mn-0.067m+0.1942n+0.3334.$$

Table 7. Edge partition of silicate chain (SL(m,n)) when m>n, m and n is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	**Number of Edges**	**(S_u,S_v) where uv ϵ E(G)**	**Number of Edges**
(12,12)	6	(27,27)	m+n-10
(15,15)	3m-6	(18,24)	2
(15,24)	m+3n+10	(18,27)	m+3n-8
(12,24)	6	(18,30)	3mn-7m-6n+12
(15,27)	m+7n-14	(24,30)	2
(24,27)	m+n+2	(27,30)	m+5n-8
(24,24)	2	(30,30)	3mn-2m-14n+4

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

SK_3 (G) $= 162mn - 39m - 96n - 144$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 7 we can apply the formula of *SK_3* index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)[12] + (m-6)[15] + (m+3n+10)[19.5] + (6)[18] + (m+7n-14)[21] +$$

$$(m+n+2)[25.5] + (2)[24] + (m+n-10)[27] + (2)[21] + (m+3n-8)[22.5] +$$

$$(3mn-7m-6n+12)[24] + (2)[27] + (m+5n-8)[28.5] + (3mn-2m-14n+4)[30]$$

$$= 162mn - 39m - 96n - 144.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

AG_2 (G) $= 6.096mn + 8.123m + 0.1642n - 9.8634$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 7 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (m-6) + (m+3n+10)[1.027] + (6)[1.060] + (m+7n-14)[1.043] + (m+n+2)[1.0017) +$$

$$(2) + (m+n-10)[1] + (2)[1.010] + (m+3n-8)[1.02] + (3mn-7m-6n+12)[1.032] + (2)[1.0062] +$$

$$(m+5n-8)[1.0013] + (3mn-2m-14n+4)$$

$$= 6.096mn + 8.123m + 0.1642n - 9.8634.$$

Table 8. Edge partition of silicate chain (SL(m,n)) when m>n, m and n is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-10
(15,15)	3n	(18,24)	2
(15,24)	m+3n+10	(18,27)	m+3n-8
(12,24)	6	(18,30)	3mn-2m-11n+2
(15,27)	m+7n-14	(24,30)	2
(24,27)	m+n+2	(27,30)	m+5n-8
(24,24)	2	(30,30)	3mn-4m-12n+8

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

SK₃ (G) $= 162mn - 24m - -156n - 114$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 8 we can apply the formula of *SK₃* index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)\left[12\right] + (3n)[15] + (m+3n+10)[19.5] + (6)[18] + (m+7n-14)[21] +$$
$$(m+n+2)[25.5] + (2)[24] + (m+n-10)[27] + (2)[21] + (m+3n-8)[22.5] +$$
$$(3mn-2m-11n+2)[24] + (2)[27] + (m+5n-8)[28.5] + (3mn-4m-12n+8)[30]$$
$$= 162mn - 24m - -156n - 114$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

AG_2 *(G)* $= 6.096mn + 3.0277m + 9.0402n + 0.0794$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 8 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u) + S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$
$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$
$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$
$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$
$$= 6 + (3n) + (m+3n+10)[1.027] + (6)[1.060] + (m+7n-14)[1.043] + (m+n+2)[1.0017) +$$
$$(2) + (m+n-10)[1] + (2)[1.010] + (m+3n-8)[1.02] + (3mn-2m-11n+2)[1.032] + (2)[1.0062] +$$
$$(m+5n-8)[1.0013] + (3mn-4m-12n+8)$$
$$= 6.096mn + 3.0277m + 9.0402n + 0.0794.$$

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest related to the publication of this article.

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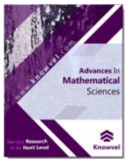

Original Research Article

ON THE INVARIANT OF NEW DEGREE-BASED TOPOLOGICAL INDICES OF SILICATE CHAIN GRAPH

Rachanna Kanabur[a] | S. K. Giregol[a] | Basavaraj M. Koujalagi[a] | Edake Yogesh Sidaraya[a]

ABSTRACT

Throughout this paper simple and undirected graphs are considered. Let G = (V, E) be such a graph. The structure of a chemical compound can be represented by a graph whose vertex and edge specify the atom and bonds respectively. In this paper we compute certain topological indices of silicate chain.

Keywords: Chemical graph, topological indices, silicate chain graph

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PUBLICATION HISTORY

Received: May 31, 2019
Accepted: June 13, 2019

ARTICLE ID: AMS-74

1. INTRODUCTION

In chemical graph theory, we have many different topological index of arbitrary molecular graph *G*. A topological index of a graphs is a member related to a graph which is invariant under graph automorphisms, obviously, every topological index defines a counting polynomial and vice versa [1, 2].

Construction of the Silicate Chain Graph:

SiO_4 tetrahedral are found nearly in all the silicates. Silicates are immensely essential and complicated minerals. We get silicate from metal carbonates with sand or from fusing metal oxides. Silicates behave as the building blocks of the usual rock-forming minerals [3]. Consider a single tetrahedron (i.e., a pyramid having a triangular base). Place oxygen atoms at the four corners of a tetrahedron, and the silicon atom is bonded with equally-spaced atoms of oxygen. The resulting tetrahedron is a silicate tetrahedron, which is shown in figure 1a, and when this tetrahedron join with other tetrahedral joins with other tetrahedral linearly, then a single-row silicate chain is formed, as shown in figure 1b. When two tetrahedral join together corner-to-corner, then each tetrahedron shares its oxygen atom with the other tetrahedron, as shown in figure 1c. After this sharing, these two tetrahedral can be joined with two other tetrahedral, as in figure 1e, were *m* is the number of row lines and *n* is the number of edges in a row line [3].

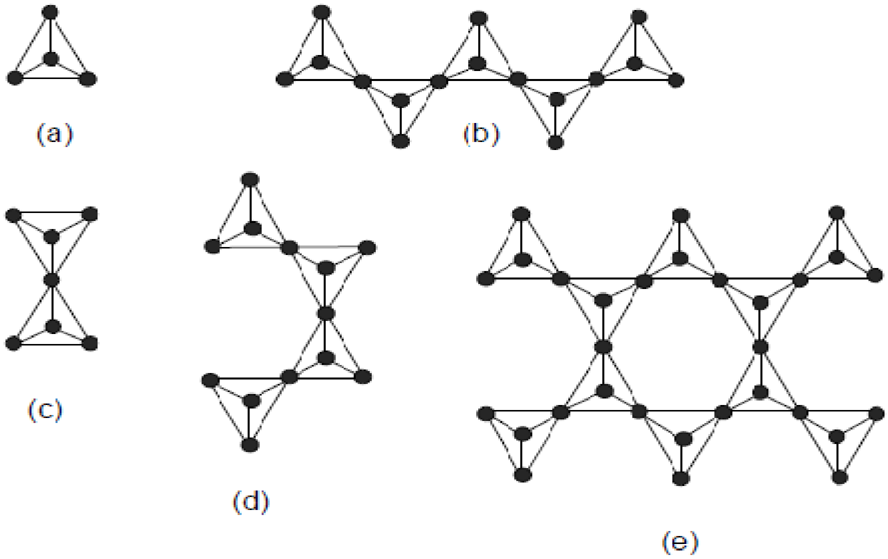

Figure 1. Chain silicate network

2. Survey of Certain Degree-Based Topological Indices

Motivated by previous research on Nanotubes [3-9], here we compute the values of two new topological indices of silicate chain.

***SK*$_3$ Index:** The SK_3 index of a graph $G = (V, E)$ is defined as,

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2} \qquad (1)$$

Where, $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbors of vertex u (or v) in G.

$S_G(u) = \sum_{u,v \in E(G)} d_G(u)$ and $N_G(u) = \{v \in V(G) / uv \in E(G)\}$

Arithmetic-Geometric (*AG*$_2$) Index: Let $G = (V, E)$ be a molecular graph, and $S_G(u)$ is the degree of the vertex u, then AG_2 index of G is defined as

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}} \qquad (2)$$

Where, $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbors of vertex u (or v) in G.

$S_G(u) = \sum_{u,v \in E(G)} d_G(u)$ and $N_G(u) = \{v \in V(G) / uv \in E(G)\}$

3. Results and Discussion

In this section, we calculate the closed results for topological indices, which based on vertex degrees of the m^{th} silicate chain. We compute the. The number of edges of the mth chain silicate are 6mn. In the following theorem, the degree-based topological indices for the m^{th} chain silicate is computed.

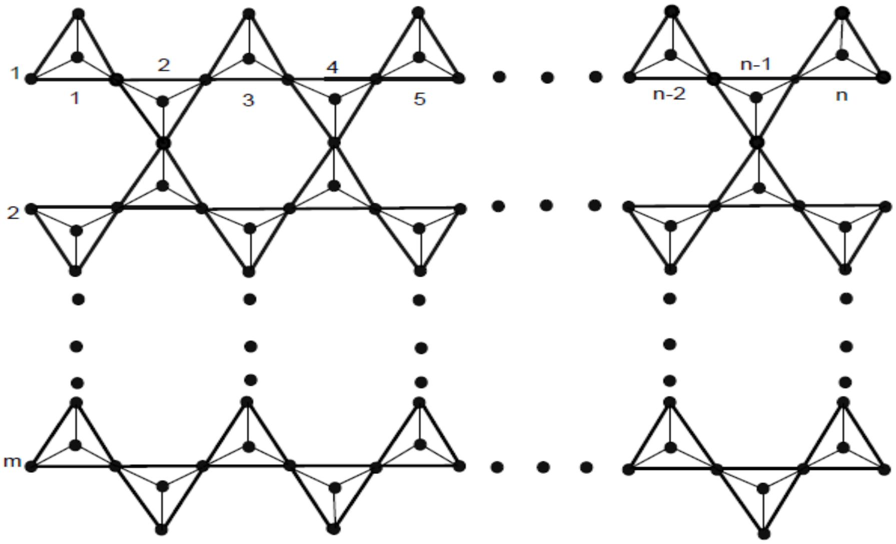

Figure 2. *m^{th}* chain silicate *(SL(m,n))*

Table 1: Edge partition of silicate chain (SL(m,n)) when m<n and m is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-7
(15,15)	3m-3	(18,24)	2
(15,24)	2m+2n+2	(18,27)	m+3n-11
(12,24)	6	(18,30)	3mn-6m-7n+16
(15,27)	m+7n-23	(24,30)	2
(24,27)	m+n-1	(27,30)	m+5n-17
(24,24)	2	(30,30)	3mn-4m-12n+26

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3(G) = 162mn - 55m - 79.5n + 52.5$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 1 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv \in E(G)} \frac{S_G(u) + S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$
$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$
$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$
$$= (6)[12] + (3m-3)[15] + (2m+2n+2)[19.5] + (6)[18] + (m+7n-23)[21] +$$
$$(m+n-1)[25.5] + (2)[24] + (m+n-7)[27] + (2)[21] + (m+3n-11)[22.5] +$$
$$(3mn-6m-7n+16)[24] + (2)[27] + (m+5n-17)[28.5] + (3mn-4m-12n+26)[30]$$
$$= 162mn - 55m - 79.5n + 52.5.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2\,(G) = 6.096mn + 0.8015m + 0.614n - 7.1893$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 1 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$
$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$
$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$
$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$
$$= 6 + (3m-3) + (2m+2n+2)[1.027] + (6)[1.060] + (m+7n-23)[1.043] + (m+n-1)[1.0017) + 2 +$$
$$(m+n-7) + (2)[1.010] + (m+3n-11)[1.02] + (3mn-6m-7n+16)[1.032] + (2)[1.0062] +$$
$$(m+5n-17)[1.0013] + (3mn-4m-12n+26)$$
$$= 6.096mn + 0.8015m + 0.614n - 7.1893.$$

Table 2. Edge partition of silicate chain (SL(m,n)) when m<n and m is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	**Number of Edges**	**(S_u,S_v) where uv ϵ E(G)**	**Number of Edges**
(12,12)	12	(27,27)	m+n-7
(15,15)	3m-6	(18,24)	4
(15,24)	m+3n-11	(18,27)	m+3n-11
(12,24)	12	(18,30)	3mn-5m-8n+18
(15,27)	m+7n-23	(24,30)	4
(24,27)	m+n-1	(27,30)	m+5n-17
(24,24)	0	(30,30)	3mn-4m-12n+26

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3(G) = 162mn - 51m - 84n + 216$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 2 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (12)\big[12\big] + (3m-6)[15] + (m+3n-11)[19.5] + (12)[18] + (m+7n-23)[21] +$$

$$(m+n-1)[25.5] + (0)[24] + (m+n-7)[27] + (4)[21] + (m+3n-11)[22.5] +$$

$$(3mn-5m-8n+18)[24] + (4)[27] + (m+5n-17)[28.5] + (3mn-4m-12n+26)[30]$$

$$= 162mn - 51m - 84n + 216\,.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2(G) = 6.096mn - 0.067m - 0.1942n + 0.0542$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 2 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right]+(15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right]+(15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right]+(12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right]+$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right]+(24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right]+(24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right]+(27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right]+$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right]+(18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right]+(18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right]+(24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right]+$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right]+(30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$=12+(3m-6)+(m+3n-11)[1.027]+(12)[1.060]+(m+7n-23)[1.043]+(m+n-1)[1.0017)+$$

$$(m+n-7)+(4)[1.010]+(m+3n-1)[1.02]+(3mn-5m-8n+18)[1.032]+(4)[1.0062]+$$

$$(m+5n-17)[1.0013]+(3mn-4m-12n+26)$$

$$=6.096mn-0.067m-0.1942n+0.0542.$$

Table 3. Edge partition of silicate chain (SL(m,n)) when m<n, m and n is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-6
(15,15)	3m-2	(18,24)	2
(15,24)	m+3n-2	(18,27)	4m-6
(12,24)	6	(18,30)	3mn+3m-16n+36
(15,27)	2m+6n-24	(24,30)	2
(24,27)	m+n-2	(27,30)	m+5n-20
(24,24)	2	(30,30)	3mn-16m+8

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

SK₃ (G) $=162mn-211.5m-4.5n-27$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 3 we can apply the formula of *SK₃* index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G)=\sum_{uv\in E(G)}\frac{S_G(u)+S_G(v)}{2}$$

$$=(12,12)\left[\frac{12+12}{2}\right]+(15,15)\left[\frac{15+15}{2}\right]+(15,24)\left[\frac{15+24}{2}\right]+(12,24)\left[\frac{12+24}{2}\right]+(15,27)\left[\frac{15+27}{2}\right]+$$

$$(24,27)\left[\frac{24+27}{2}\right]+(24,24)\left[\frac{24+24}{2}\right]+(27,27)\left[\frac{27+27}{2}\right]+(18,24)\left[\frac{18+24}{2}\right]+(18,27)\left[\frac{18+27}{2}\right]+$$

$$(18,30)\left[\frac{18+30}{2}\right]+(24,30)\left[\frac{24+30}{2}\right]+(27,30)\left[\frac{27+30}{2}\right]+(30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)\left[12\right] + (3m-2)[15] + (m+3n-2)[19.5] + (6)[18] + (2m+6n-24)[21] +$$
$$(m+n-2)[25.5] + (2)[24] + (m+n-6)[27] + (2)[21] + (4m-6)[22.5] +$$
$$(3mn+3m-16n+36)[24] + (2)[27] + (m+5n-20)[28.5] + (3mn-16m+8)[30]$$

$$= 162mn - 211.5m - 4.5n - 27\,.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2\ (G)\ = 6.096mn + 0.29m - 01648n + 0.309$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 3 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$
$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$
$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$
$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$
$$= 6 + (3m-2) + (m+3n-2)[1.027] + (6)[1.060] + (2m+6n-24)[1.043] + (m+n-2)[1.0017) +$$
$$(2) + (m+n-6)[1] + (2)[1.010] + (4m-6)[1.02] + (3mn+3m-16n+36)[1.032] + (2)[1.0062] +$$
$$(m+5n-20)[1.0013] + (3mn-16m+8)$$
$$= 6.096mn + 0.29m - 01648n + 0.309\,.$$

Table 4. Edge partition of silicate chain (SL(m,n)) when m<n , m and n is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-6
(15,15)	3m-2	(18,24)	2
(15,24)	m+3n-2	(18,27)	m+3n-12
(12,24)	6	(18,30)	3mn-13m+4
(15,27)	m+7n-26	(24,30)	2
(24,27)	m+n-2	(27,30)	m+5n-20
(24,24)	2	(30,30)	3mn+4m-20n+48

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3\ (G)\ = 162mn - 3m - 132n + 192$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 4 we can apply the formula of *SK₃* index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv \in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)[12] + (3m-2)[15] + (m+3n-2)[19.5] + (6)[18] + (m+7n-26)[21] +$$

$$(m+n-2)[25.5] + (2)[24] + (m+n-6)[27] + (2)[21] + (m+3n-12)[22.5] +$$

$$(3mn-13m+4)[24] + (2)[27] + (m+5n-20)[28.5] + (3mn+4m-20n+48)[30]$$

$$= 162mn - 3m - 132n + 192.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

AG₂ (G) $= 6.096mn - 0.323m + 0.4502n + 1.079$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m<n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 4 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv \in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (3m-2) + (m+3n-2)[1.027] + (6)[1.060] + (m+7n-26)[1.043] + (m+n-2)[1.0017) +$$

$$(2) + (m+n-6)[1] + (2)[1.010] + (m+3n-12)[1.02] + (3mn-13m+4)[1.032] + (2)[1.0062] +$$

$$(m+5n-20)[1.0013] + (3mn+4m-20n+48)$$

$$= 6.096mn - 0.323m + 0.4502n + 1.079.$$

Table 5. Edge partition of silicate chain (SL(m,n)) when m>n m is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-9
(15,15)	m+2n-3	(18,24)	2
(15,24)	m+3n+7	(18,27)	m+3n-9
(12,24)	6	(18,30)	3mn-5m-8n+11
(15,27)	m+7n-17	(24,30)	2
(24,27)	m+n+1	(27,30)	m+5n-11
(24, 24)	2	(30,30)	3mn-2m-14n+12

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3\,(G)\ = 162mn - 21m - 181.5n - 29$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 5 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)\left[12\right] + (m+2n-3)[15] + (m+3n-2)[19.5] + (6)[18] + (m+7n-17)[21] +$$

$$(m+n+1)[25.5] + (2)[24] + (m+n-9)[27] + (2)[21] + (m+3n-9)[22.5] +$$

$$(3mn-5m-8n+1)[24] + (2)[27] + (m+5n-11)[28.5] + (3mn-2m-14n+12)[30]$$

$$= 162mn - 21m - 181.5n - 29\,.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2\,(G)\ = 6.096mn - 0.067m + 0.1942n + 9.8 * 10^{-03}$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 5 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n))

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (m+2n-3) + (m+3n+7)[1.027] + (6)[1.060] + (m+7n-17)[1.043] + (m+n+1)[1.0017) +$$

$$(2) + (m+n-9)[1] + (2)[1.010] + (m+3n-9)[1.02] + (3mn-5m-8n+1)[1.032] + (2)[1.0062] +$$

$$(m+5n-11)[1.0013] + (3mn-2m-14n+12)$$

$$= 6.096mn - 0.067m + 0.1942n + 9.8*10^{-03}$$

Table 6. Edge partition of silicate chain (SL(m,n)) when m>n and m is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	12	(27,27)	m+n-9
(15,15)	m+2n-6	(18,24)	4
(15,24)	m+3n-5	(18,27)	m+3n-9
(12,24)	12	(18,30)	3mn-5m-8n+12
(15,27)	m+7n-17	(24,30)	4
(24,27)	m+n+1	(27,30)	m+5n-11
(24,24)	0	(30,30)	3mn-2m-14n+12

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3(G) = 162mn - 21m + 264n + 29.5$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 6 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G)=\sum_{uv\in E(G)}\frac{S_G(u)+S_G(v)}{2}$$

$$=(12,12)\left[\frac{12+12}{2}\right]+(15,15)\left[\frac{15+15}{2}\right]+(15,24)\left[\frac{15+24}{2}\right]+(12,24)\left[\frac{12+24}{2}\right]+(15,27)\left[\frac{15+27}{2}\right]+$$

$$(24,27)\left[\frac{24+27}{2}\right]+(24,24)\left[\frac{24+24}{2}\right]+(27,27)\left[\frac{27+27}{2}\right]+(18,24)\left[\frac{18+24}{2}\right]+(18,27)\left[\frac{18+27}{2}\right]+$$

$$(18,30)\left[\frac{18+30}{2}\right]+(24,30)\left[\frac{24+30}{2}\right]+(27,30)\left[\frac{27+30}{2}\right]+(30,30)\left[\frac{30+30}{2}\right]$$

$$=(6)[12]+(m+2n-6)[15]+(m+3n-5)[19.5]+(12)[18]+(m+7n-17)[21]+$$

$$(m+n+1)[25.5]+(0)[24]+(m+n-9)[27]+(4)[21]+(m+3n-9)[22.5]+$$

$$(3mn-5m-8n+12)[24]+(4)[27]+(m+5n-11)[28.5]+(3mn-2m-14n+12)[30]$$

$$=162mn-21m+264n+29.5.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$$AG_2\ (G)\ =6.096mn-0.067m+0.1942n+0.3334$$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n and m is even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 6 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G)=\sum_{uv\in E(G)}\frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$=(12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right]+(15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right]+(15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right]+(12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right]+$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right]+(24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right]+(24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right]+(27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right]+$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right]+(18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right]+(18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right]+(24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right]+$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right]+(30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$=21+(m+2n-6)+(m+3n-5)[1.027]+(12)[1.060]+(m+7n-17)[1.043]+(m+n+1)[1.0017)+$$

$$(0)+(m+n-9)[1]+(4)[1.010]+(m+3n-9)[1.02]+(3mn-5m-8n+12)[1.032]+(4)[1.0062]+$$

$$(m+5n-11)[1.0013]+(3mn-2m-14n+12)$$

$$=6.096mn-0.067m+0.1942n+0.3334.$$

Table 7. Edge partition of silicate chain (SL(m,n)) when m>n, m and n is even, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	**Number of Edges**	**(S_u,S_v) where uv ϵ E(G)**	**Number of Edges**
(12,12)	6	(27,27)	m+n-10
(15,15)	3m-6	(18,24)	2
(15,24)	m+3n+10	(18,27)	m+3n-8
(12,24)	6	(18,30)	3mn-7m-6n+12
(15,27)	m+7n-14	(24,30)	2
(24,27)	m+n+2	(27,30)	m+5n-8
(24,24)	2	(30,30)	3mn-2m-14n+4

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3(G) = 162mn - 39m - 96n - 144$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 7 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$= (6)\left[12\right] + (m-6)[15] + (m+3n+10)[19.5] + (6)[18] + (m+7n-14)[21] +$$

$$(m+n+2)[25.5] + (2)[24] + (m+n-10)[27] + (2)[21] + (m+3n-8)[22.5] +$$

$$(3mn-7m-6n+12)[24] + (2)[27] + (m+5n-8)[28.5] + (3mn-2m-14n+4)[30]$$

$$= 162mn - 39m - 96n - 144.$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$AG_2(G) = 6.096mn + 8.123m + 0.1642n - 9.8634$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are even, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 7 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u)+S_G(v)}}$$

$$= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] +$$

$$(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] +$$

$$(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] +$$

$$(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right]$$

$$= 6 + (m-6) + (m+3n+10)[1.027] + (6)[1.060] + (m+7n-14)[1.043] + (m+n+2)[1.0017) +$$

$$(2) + (m+n-10)[1] + (2)[1.010] + (m+3n-8)[1.02] + (3mn-7m-6n+12)[1.032] + (2)[1.0062] +$$

$$(m+5n-8)[1.0013] + (3mn-2m-14n+4)$$

$$= 6.096mn + 8.123m + 0.1642n - 9.8634.$$

Table 8. Edge partition of silicate chain (SL(m,n)) when m>n, m and n is odd, based on the sum degrees of the end vertices of each edge

(S_u,S_v) where uv ϵ E(G)	Number of Edges	(S_u,S_v) where uv ϵ E(G)	Number of Edges
(12,12)	6	(27,27)	m+n-10
(15,15)	3n	(18,24)	2
(15,24)	m+3n+10	(18,27)	m+3n-8
(12,24)	6	(18,30)	3mn-2m-11n+2
(15,27)	m+7n-14	(24,30)	2
(24,27)	m+n+2	(27,30)	m+5n-8
(24,24)	2	(30,30)	3mn-4m-12n+8

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

$SK_3(G) = 162mn - 24m - -156n - 114$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 8 we can apply the formula of SK_3 index to compute this index for silicate chain (SL(m,n)).

$$SK_3(G) = \sum_{uv \in E(G)} \frac{S_G(u) + S_G(v)}{2}$$

$$= (12,12)\left[\frac{12+12}{2}\right] + (15,15)\left[\frac{15+15}{2}\right] + (15,24)\left[\frac{15+24}{2}\right] + (12,24)\left[\frac{12+24}{2}\right] + (15,27)\left[\frac{15+27}{2}\right] +$$

$$(24,27)\left[\frac{24+27}{2}\right] + (24,24)\left[\frac{24+24}{2}\right] + (27,27)\left[\frac{27+27}{2}\right] + (18,24)\left[\frac{18+24}{2}\right] + (18,27)\left[\frac{18+27}{2}\right] +$$

$$(18,30)\left[\frac{18+30}{2}\right] + (24,30)\left[\frac{24+30}{2}\right] + (27,30)\left[\frac{27+30}{2}\right] + (30,30)\left[\frac{30+30}{2}\right]$$

$$
\begin{aligned}
&= (6)\left[12\right] + (3n)[15] + (m+3n+10)[19.5] + (6)[18] + (m+7n-14)[21] + \\
&(m+n+2)[25.5] + (2)[24] + (m+n-10)[27] + (2)[21] + (m+3n-8)[22.5] + \\
&(3mn-2m-11n+2)[24] + (2)[27] + (m+5n-8)[28.5] + (3mn-4m-12n+8)[30] \\
&= 162mn - 24m - -156n - 114
\end{aligned}
$$

Theorem: Let G be a graph of silicate chain (SL(m,n)), then

AG₂ (G) $= 6.096mn + 3.0277m + 9.0402n + 0.0794$

Proof: We use the edge partition of graph of silicate chain (SL(m,n)), when m>n, m and n both are odd, based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 8 we can apply the formula of Arithmetic-Geometric index to compute this index for silicate chain (SL(m,n)).

$$AG_2(G) = \sum_{uv \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u) + S_G(v)}}$$

$$
\begin{aligned}
&= (12,12)\left[\frac{12+12}{2\sqrt{12*12}}\right] + (15,15)\left[\frac{15+15}{2\sqrt{15*15}}\right] + (15,24)\left[\frac{15+24}{2\sqrt{15*24}}\right] + (12,24)\left[\frac{12+24}{2\sqrt{12*24}}\right] + \\
&(15,27)\left[\frac{15+27}{2\sqrt{15*27}}\right] + (24,27)\left[\frac{24+27}{2\sqrt{24*27}}\right] + (24,24)\left[\frac{24+24}{2\sqrt{24*24}}\right] + (27,27)\left[\frac{27+27}{2\sqrt{27*27}}\right] + \\
&(18,24)\left[\frac{18+24}{2\sqrt{18*24}}\right] + (18,27)\left[\frac{18+27}{2\sqrt{18*27}}\right] + (18,30)\left[\frac{18+30}{2\sqrt{18*30}}\right] + (24,30)\left[\frac{24+30}{2\sqrt{24*30}}\right] + \\
&(27,30)\left[\frac{27+30}{2\sqrt{27*30}}\right] + (30+30)\left[\frac{30+30}{2\sqrt{30*30}}\right] \\
&\qquad = 6 + (3n) + (m+3n+10)[1.027] + (6)[1.060] + (m+7n-14)[1.043] + (m+n+2)[1.0017) + \\
&\qquad (2) + (m+n-10)[1] + (2)[1.010] + (m+3n-8)[1.02] + (3mn-2m-11n+2)[1.032] + (2)[1.0062] + \\
&\qquad (m+5n-8)[1.0013] + (3mn-4m-12n+8) \\
&= 6.096mn + 3.0277m + 9.0402n + 0.0794.
\end{aligned}
$$

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest related to the publication of this article.

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GLOBAL JOURNAL OF APPLIED ENGINEERING MATHEMATICS
Vol. 01 (2019) 14-34
www.knowvel.com

Original Research Article

ON COMPUTATION OF NEW DEGREE-BASED TOPOLOGICAL INDICES OF SILICATE CHAIN GRAPH

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ABSTRACT

The Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2 indices of a graph G was introduced by V. S. Shigehalli and R. R. Kanabur. These topological indices explain the modeling of various physico-chemical, biological and pharmacological properties of organic molecules in chemistry and explains studies of various results on Silicate Chain Graph.

Keywords: Molecular graph, arithmetic-geometric index (AG_1 index), SK index, SK_1 index, SK_2 index, silicate chain graph

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PUBLICATION HISTORY

Received: May 31, 2019
Accepted: June 12, 2019

ARTICLE ID: GJAEM-73

1. INTRODUCTION

In chemical graph theory, we have many different topological index of arbitrary molecular graph *G*. A topological index of a graphs is a member related to a graph which is invariant under graph automorphisms, obviously, every topological index defines a counting polynomial and vice versa [1, 2].

Construction of the Silicate Chain Graph:

SiO_4 tetrahedral are found nearly in all the silicates. Silicates are immensely essential and complicated minerals. We get silicate from metal carbonates with sand or from fusing metal oxides. Silicates behave as the building blocks of the usual rock-forming minerals [3]. Consider a single tetrahedron (i.e., a pyramid having a triangular base). Place oxygen atoms at the four corners of a tetrahedron, and the silicon atom is bonded with equally-spaced atoms of oxygen. The resulting tetrahedron is a silicate tetrahedron, which is shown in figure 1a, and when this tetrahedron join with other tetrahedral joins with other tetrahedral linearly, then a single-row silicate chain is formed, as shown in figure 1b. When two tetrahedral join together corner-to-corner, then each tetrahedron shares its oxygen atom with the other tetrahedron, as shown in figure 1c. After this sharing, these two tetrahedral can be joined with two other tetrahedral, as in figure 1e, were m is the number of row lines and n is the number of edges in a row line [3].

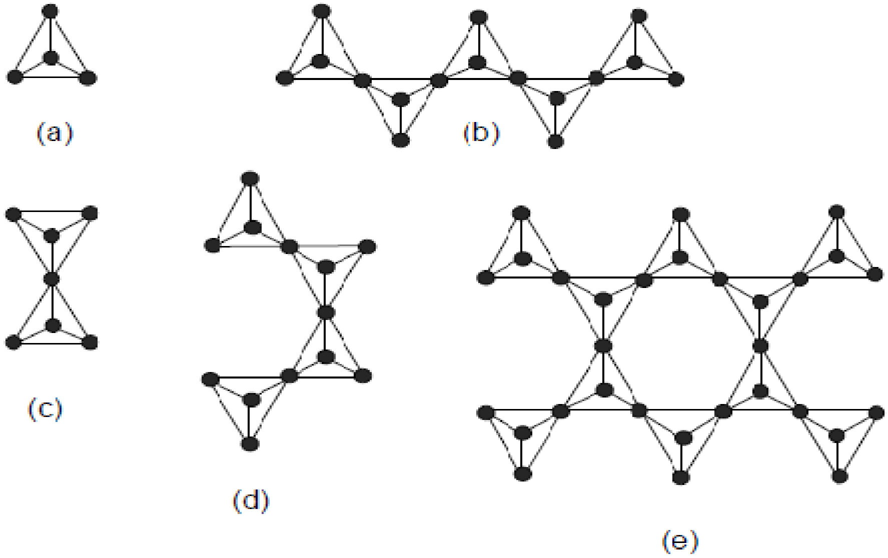

Figure 1. Chain silicate network

2. Survey of Certain Degree-Based Topological Indices

Motivated by previous research on Nanotubes [3-9], here we compute the values of four new topological indices of silicate chain.

Arithmetic-Geometric (*AG_1*) Index: Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u, then AG_1 index of G is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}} \qquad (1)$$

Where, AG_1 index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

***SK* Index:** The SK index of a graph $G = (V, E)$ is defined as,

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2} \qquad (2)$$

Where, $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

***SK_1* Index:** The SK_1 index of a graph $G = (V, E)$ is defined as,

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2} \qquad (3)$$

Where, $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

***SK_2* Index:** The SK_2 index of a graph $G = (V, E)$ is defined as,

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2 \qquad (4)$$

Where, $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

3. RESULTS AND DISCUSSION

In this section, we calculate the closed results for topological indices, which based on vertex degrees of the m^{th} silicate chain. We compute the. The number of edges of the m^{th} chain silicate are 6mn. In the following theorem, the degree-based topological indices for the m^{th} chain silicate is computed.

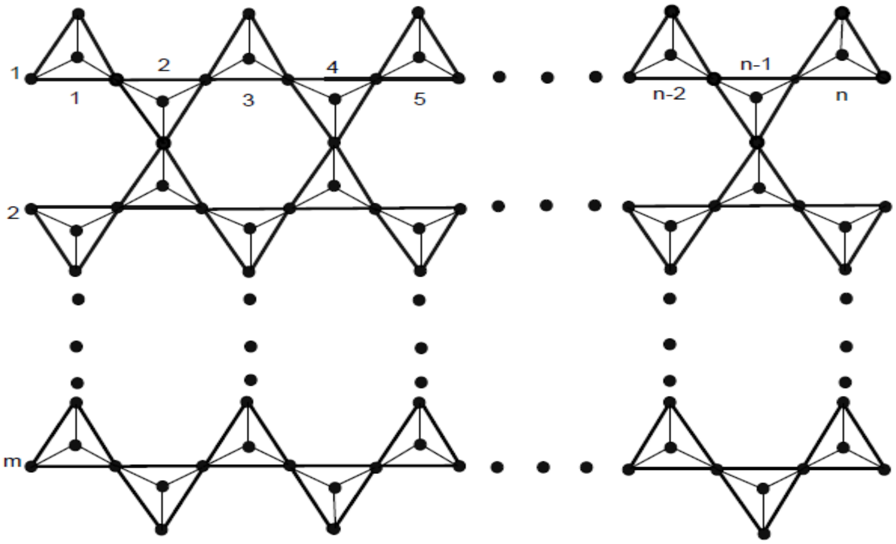

Figure 2. m^{th} chain silicate *(SL(m,n))*

Table 1. Edge partition of silicate chain (SL(m,n)) when m=n based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	**Number of Edges**
(3,3)	3m+2
(3,6)	3mn+3n-4
(6,6)	3mn-6n+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+3m+21n-0.242$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.1 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+2)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+3n-4)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-6n+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=3m+2+\left[\frac{1}{2\sqrt{18}}\right](27mn+27n-36)+3mn-6n+2$$

$$=3mn+3m-6n+4+\left[\frac{1}{2\sqrt{18}}\right](27mn+27n-36)$$

$$=6.18mn+3m+21n-0.242$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn+9m-22.5n$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.1 we compute the SK index of G which is expressed as

SK(G) = $\sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+2)[3]+(3mn+3n-4)\left[\frac{9}{2}\right]+(3mn-6n+2)[6]$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+2)[3]+(3mn+3n-4)\left[\frac{9}{2}\right]+(3mn-6n+2)[6]$$

$$=18mn+9m-36n+18+\frac{1}{2}[27mn-36n-36]$$

$$=31.5mn+9m-22.5n$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_1$ index is equal to

SK$_1$ (SL(m,n)) = $13.5m+9+81mn-81n$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK$_1$ index of G which is expressed as

SK$_1$(G) = $\sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+2)\left[\frac{9}{2}\right]+(3mn+3n-4)[9]+(3mn-6n+2)[18]$$

$$=\frac{1}{2}[27m+18]+27mn+27n-36+54mn-108n+36$$

$$=\frac{1}{2}[27m+18]+81mn-81n$$

$$=13.5m+9+81mn-81n$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_2$ index is equal to

SK$_2$ (SL(m,n)) = $168.75mn+27m-155.25n+9$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.1 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2} \right)^2$$

$$= (3,3)\left[\frac{3+3}{2}\right]^2 + (3,6)\left[\frac{3+6}{2}\right]^2 + (6,6)\left[\frac{6+6}{2}\right]^2$$

$$= (3m+2)[3]^2 + (3mn+3n-4)\left[\frac{9}{2}\right]^2 + (3mn-6n+2)[6]^2$$

$$= 27m+18+\frac{1}{4}[3mn+3n-4]+108mn-216n+72$$

$$= 108mn-27m-216n+90+\left[\frac{1}{4}\right](27mn+9m+18n-54)$$

$$= 168.75mn+27m-155.25n+9$$

Table 2. Edge partition of silicate chain (SL(m,n)) when m<n and m is odd based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	**Number of Edges**
(3,3)	3m+3
(3,6)	3mn+m+2n-5
(6,6)	3mn-2n-4m+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $12.18mn-7.94m-3.88n+0.697$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right] + (3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right] + (6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+3)\left[\frac{6}{2\sqrt{9}}\right] + (3mn+m+2n-5)\left[\frac{9}{2\sqrt{18}}\right] + (3mn-2n-4m+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-45)+3m+3+9mn-6n-12m+6$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-45)+9mn-9m-6n+9$$

$$= 12.18mn-7.94m-3.88n+0.697$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn - 1.5m - 12n - 1.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+3)[3]+(3mn+m+2n-5)\left[\frac{9}{2}\right]+(3mn-2n-4m+2)[6]$$

$$=18mn-15m-12n+21+\left[\frac{1}{2}\right](27mn+9m+18m-45)$$

$$=31.5mn-1.5m-12n-1.5$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_1$ index is equal to

SK$_1$ (SL(m,n)) = $81mn - 51.5m - 54n + 4.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the SK$_1$ index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+3)\left[\frac{9}{2}\right]+(3mn+m-2n-5)[9]+(3mn-2n-4m+2)[18]$$

$$=\frac{1}{2}[27m+27]+27mn+9m-18n-45+54mn-36n-72m+36$$

$$=\frac{1}{2}[27m+27]+81mn-65m-54n-9$$

$$=81mn-51.5m-54n+4.5$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_2$ index is equal to

SK$_2$ (SL(m,n)) = $168.75mn - 96.75m - 31.5n + 2.25$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the SK$_2$ index of G which is expressed as

$$SK_2\,(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+3)[3]^2+(3mn+m+2n-5)\left[\frac{9}{2}\right]^2+(3mn-2n-4m+2)[6]^2$$

$$=27m+27+\frac{1}{4}[243mn+81m+162n-405]+108mn-72n-144m+72$$

$$=108mn-117m-72n+99+\left[\frac{1}{4}\right](243mn+81m+162n-405)$$

$$=168.75mn-96.75m-31.5n+2.25$$

Table 3. Edge partition of silicate chain (SL(m,n)) when m<n and m is even, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+6
(3,6)	3mn+m+2n-8
(6,6)	3mn-2n-4m+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn-0.06m+0.12n-0.48$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=(3m+6)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+m+2n-8)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2n-4m+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-72)+3mn-m-2n+8$$

$$=6.18mn-0.06m+0.12n-0.48$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn-10.5m-3n-6$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the SK index of G which is expressed as

$$SK(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=\left(3m+3\right)\left[3\right]+(3mn+m+2n-5)\left[\frac{9}{2}\right]+\left(3mn-2n-4m+2\right)\left[6\right]$$

$$=18mn-15m-12n+30+\left[\frac{1}{2}\right]\left(27mn+9m+18m-72\right)$$

$$=31.5mn-10.5m-3n-6$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $8mn-49.5m-18n-9$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G\left(u\right).d_G\left(v\right)}{2}$$

$$=\left(3,3\right)\left[\frac{3.3}{2}\right]+\left(3,6\right)\left[\frac{3.6}{2}\right]+\left(6,6\right)\left[\frac{6.6}{2}\right]$$

$$=\left(3m+6\right)\left[\frac{9}{2}\right]+(3mn+m-2n-8)\left[9\right]+\left(3mn-2n-4m+2\right)\left[18\right]$$

$$=\left[\frac{1}{2}\right]\left(27m+54\right)+27mn+9m+18n-72+54mn-36n-72m+36$$

$$=\left[\frac{1}{2}\right]\left(27m+54\right)+8mn-63m-18n-36$$

$$=8mn-49.5m-18n-9$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $168.75mn-96.75m-31.5n-36$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the SK_2 index of G which is expressed as

$$SK_2\,(G) = \sum_{u,v\in E(G)} \left(\frac{d_G\left(u\right)+d_G\left(v\right)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+6)[3]^2+(3mn+m+2n-8)\left[\frac{9}{2}\right]^2+(3mn-2n-4m+2)[6]^2$$

$$=27m+54+\left[\frac{1}{4}\right]\left(243mn+81m+162n-648\right)+108mn-72n-144m+72$$

$$=108mn-72n-117m+126+\left[\frac{1}{4}\right](243mn+81m+162n-648)$$

$$=168.75mn-96.75m-31.5n-36$$

Table 4. Edge partition of silicate chain (SL(m,n)) when m<n and m & n both are even, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+4
(3,6)	3mn+m+2n-6
(6,6)	3mn-4m-2n+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+0.06m+0.12n-0.36$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=(3m+4)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+m+2n-6)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-4m-2n+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-m-2n+6$$

$$=6.18mn+0.06m+0.12n-0.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn-10.5m-3n-3$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+4)[3]+(3mn+m+2n-6)\left[\frac{9}{2}\right]+(3mn-4m-2n+2)[6]$$

$$=18mn-15m-12n+24+\left[\frac{1}{2}\right](27mn+9m+18n-54)$$

$$=31.5mn-10.5m-3n-3$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn - 49.5m - 18n$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$= (3,3)\left[\frac{3.3}{2}\right] + (3,6)\left[\frac{3.6}{2}\right] + (6,6)\left[\frac{6.6}{2}\right]$$

$$= (3m+4)\left[\frac{9}{2}\right] + (3mn + m + 2n - 6)[9] + (3mn - 4m - 2n + 2)[18]$$

$$= \left[\frac{1}{2}\right](27m + 36) + 27mn + 9m - 18n - 54 + 54mn - 72m - 36n + 36$$

$$= \left[\frac{1}{2}\right](27m + 36) + 81mn - 63m - 18n - 18$$

$$= 81mn - 49.5m - 18n$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $114.75mn - 114.75m - 67.5n + 94.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the SK_2 index of G which is expressed as

$$SK_2\,(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2$$

$$= (3,3)\left[\frac{3+3}{2}\right]^2 + (3,6)\left[\frac{3+6}{2}\right]^2 + (6,6)\left[\frac{6+6}{2}\right]^2$$

$$= (3m+4)[3]^2 + (3mn + m + 2n - 6)\left[\frac{9}{2}\right]^2 + (3mn - 4m - 2n + 2)[6]^2$$

$$= 27m + 36 + \left[\frac{1}{4}\right](27mn + 9m + 18n - 54) + 108mn - 144m - 72n + 72$$

$$= 108mn - 117m - 72n + 108 + \left[\frac{1}{4}\right](27mn + 9m + 18n - 54)$$

$$= 114.75mn - 114.75m - 67.5n + 94.5$$

Table 5. Edge partition of silicate chain (SL(m,n)) when m<n and m & n both are odd, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+4
(3,6)	3mn+3m-2
(6,6)	3mn-6m-2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+0.18m-4.12$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+4)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+3m-2)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-6m-2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=(3m+4)[1]+\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-6m-2$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-3m-2$$

$$=6.18mn+0.18m-4.12$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn+4.5m-9$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+4)[3]+(3mn+3m-2)\left[\frac{9}{2}\right]+(3mn-6m-2)[6]$$

$$= \quad 9m+12+\left[\frac{1}{2}\right](27mn+27m-18)+18mn-36m-12$$

$$=\left[\frac{1}{2}\right](27mn+27m-18)+18mn-27m$$

$$=31.5mn+4.5m-9$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn-67.5m-36$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+4)\left[\frac{9}{2}\right]+(3mn+m+2n-6)[9]+(3mn-4m-2n+2)[18]$$

$$=\left[\frac{1}{2}\right](27m+36)+27mn+9m-18n-54+54mn-72m-36n+36$$

$$=\left[\frac{1}{2}\right](27m+36)+81mn-63m-18n-18$$

$$=81mn-67.5m-36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $168.75mn-148.5m-76.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the SK_2 index of G which is expressed as

$$SK_2\ (G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+4)[3]^2+(3mn+m+2n-6)\left[\frac{9}{2}\right]^2+(3mn-4m-2n+2)[6]^2$$

$$=27m+36+\left[\frac{1}{4}\right](27mn+9m+18n-54)+108mn-144m-72n+72$$

$$=108mn-117m-72n+108+\left[\frac{1}{4}\right](27mn+9m+18n-54)$$

$$=168.75mn-148.5m-76.5$$

Table 6. Edge partition of silicate chain (SL(m,n)) when m>n and m is odd, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+1
(3,6)	3mn-m+4n-1
(6,6)	3mn-2m-4n

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn-1.94m+2.12n-7.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=(3m+1)\left[\frac{6}{2\sqrt{9}}\right]+(3mn-m+4n-1)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2m-4n)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=(3m+1)[1]+\left[\frac{1}{2\sqrt{18}}\right](27mn-m+4n-1)+3mn-6m-2$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-3m-1$$

$$=6.18mn-1.94m+2.12n-7.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $19.5mn-3.5m-22n+2.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+1)[3]+(3mn-m+4n-1)\left[\frac{9}{2}\right]+(3mn-2m-4n)[6]$$

$$= 9m+3+\left[\frac{1}{2}\right](3mn-m+4n-1)+18mn-12m-24n$$

$$=\left[\frac{1}{2}\right](3mn-m+4n-1)+18mn-3m-24n+3$$

$$=19.5mn-3.5m-22n+2.5$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_1$ index is equal to

SK$_1$ (SL(m,n)) = $81mn-31.5m-36n+9$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the SK$_1$ index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+1)\left[\frac{9}{2}\right]+(3mn-m+4n-1)[9]+(3mn-2m-4n)[18]$$

$$=\left[\frac{1}{2}\right](27m+36)+27mn-9m+36n-9+54mn-36m-72n$$

$$=\left[\frac{1}{2}\right](27m+36)+81mn-45m-36n-9$$

$$=81mn-31.5m-36n+9$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_2$ index is equal to

SK$_2$ (SL(m,n)) = $87.75mn-42.75m-139.5n-4.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the SK$_2$ index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+1)[3]^2+(3mn-m+4n-1)\left[\frac{9}{2}\right]^2+(3mn-2m-4n)[6]^2$$

$$=27m+9+\left[\frac{1}{4}\right](27mn+9m+18n-54)+108mn-72m-144n$$

$$=108mn-45m-144n+9+\left[\frac{1}{4}\right](27mn+9m+18n-54)$$

$$=87.75mn-42.75m-139.5n-4.5$$

Table 7. Edge partition of silicate chain (SL(m,n)) when m>n and m is even, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+4
(3,6)	3mn-m+4n-4
(6,6)	3mn-2m-4n

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+2.060m-1.88n-2.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+4)\left[\frac{6}{2\sqrt{9}}\right]+(3mn-m+4n-4)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2m-4n)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= (3m+4)[1]+\left[\frac{1}{2\sqrt{18}}\right](3mn-m+4n-4)+3mn-2m-4n$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn+m-4n+4$$

$$= 6.18mn+2.060m-1.88n-2.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn-7.5m-6n-6$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$= (3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$= (3m+4)[3]+(3mn-m+4n-4)\left[\frac{9}{2}\right]+(3mn-2m-4n)[6]$$

$$= \quad 9m+12+\left[\frac{1}{2}\right](27mn-9m+36n-36)+18mn-12m-24n$$

$$= \left[\frac{1}{2}\right](27mn-9m+36n-36)+18mn-3m-24n+12$$

$$= 31.5mn - 7.5m - 6n - 6$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn - 31.5m + 36n - 90$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$= (3,3)\left[\frac{3.3}{2}\right] + (3,6)\left[\frac{3.6}{2}\right] + (6,6)\left[\frac{6.6}{2}\right]$$

$$= (3m+4)\left[\frac{9}{2}\right] + (3mn - m + 4n - 4)[9] + (3mn - 2m - 4n)[18]$$

$$= \left[\frac{1}{2}\right](27m+36) + 27mn - 9m + 36n - 36 + 54mn - 36m - 72$$

$$= \left[\frac{1}{2}\right](27m+36) + 81mn - 45m + 36n - 108$$

$$= 81mn - 31.5m + 36n - 90$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $114.75mn - 42.75m - 139.5n + 22.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the SK_2 index of G which is expressed as

$$SK_2\,(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2$$

$$= (3,3)\left[\frac{3+3}{2}\right]^2 + (3,6)\left[\frac{3+6}{2}\right]^2 + (6,6)\left[\frac{6+6}{2}\right]^2$$

$$= (3m+4)[3]^2 + (3mn - m + 4n - 4)\left[\frac{9}{2}\right]^2 + (3mn - 2m - 4n)[6]^2$$

$$= 27m + 36 + \left[\frac{1}{4}\right](3mn - m + 4n - 4) + 108mn - 72m - 144n$$

$$= 108mn - 45m - 144n + 36 + \left[\frac{1}{4}\right](27mn + 9m + 18n - 54)$$

$$= 114.75mn - 42.75m - 139.5n + 22.5$$

Table 8. Edge partition of silicate chain (SL(m,n)) when m>n and m & n both are even, based on the degrees of the end vertices of each edge.

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m
(3,6)	3mn-m+4n+2
(6,6)	3mn-2m-4n-2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+2.060m-1.88n-8.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m)\left[\frac{6}{2\sqrt{9}}\right]+(3mn-m+4n+2)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2m-4n-2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= (3m)[1]+\left[\frac{1}{2\sqrt{18}}\right](3mn-m+4n+2)+3mn-2m-4n-2$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn+m-4n-2$$

$$= 6.18mn+2.060m-1.88n-8.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $94.5mn-7.5m-6n-3$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$= (3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$= (3m)[3]+(3mn-m+4n+2)\left[\frac{9}{2}\right]+(3mn-2m-4n-2)[6]$$

$$= 9m+\left[\frac{1}{2}\right](27mn-9m+36n+18)+18mn-12m-24n-12$$

$$= \left[\frac{1}{2}\right](27mn-9m+36n+18)+18mn-3m-24n-12$$

$$=94.5mn-7.5m-6n-3$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn-31.5m-36n-18$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m)\left[\frac{9}{2}\right]+(3mn-m+4n+2)[9]+(3mn-2m-4n-2)[18]$$

$$=\left[\frac{1}{2}\right](27m)+27mn-9m+36n+18+54mn-36m-72n-36$$

$$=\left[\frac{1}{2}\right](27m)+81mn-45m-36n-18$$

$$=81mn-31.5m-36n-18$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $108mn-45.5m-143n-71.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m)[3]^2+(3mn-m+4n+2)\left[\frac{9}{2}\right]^2+(3mn-2m-4n-2)[6]^2$$

$$=27m+\left[\frac{1}{4}\right](3mn-m+4n+2)+108mn-72m-144n-72$$

$$=\left[\frac{1}{4}\right](3mn-m+4n+2)+108mn-45m-144n-72$$

$$=108mn-45.5m-143n-71.5$$

Table 9. Edge partition of silicate chain (SL(m,n)) when m>n and m & n both are odd, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m
(3,6)	3mn-m+4n+2
(6,6)	3mn-2m-4n-2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn + 2.060m - 1.88n - 8.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right] + (3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right] + (6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m)\left[\frac{6}{2\sqrt{9}}\right] + (3mn - m + 4n + 2)\left[\frac{9}{2\sqrt{18}}\right] + (3mn - 2m - 4n - 2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= (3m)[1] + \left[\frac{1}{2\sqrt{18}}\right](3mn - m + 4n + 2) + 3mn - 2m - 4n - 2$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn + 9m + 18n - 54) + 3mn + m - 4n - 2$$

$$= 6.18mn + 2.060m - 1.88n - 8.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK(SL(m,n)) = $94.5mn - 7.5m - 6n - 3$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the SK index of G which is expressed as

$$SK(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$= (3,3)\left[\frac{3+3}{2}\right] + (3,6)\left[\frac{3+6}{2}\right] + (6,6)\left[\frac{6+6}{2}\right]$$

$$= (3m)[3] + (3mn - m + 4n + 2)\left[\frac{9}{2}\right] + (3mn - 2m - 4n - 2)[6]$$

$$= \quad 9m + \left[\frac{1}{2}\right](27mn - 9m + 36n + 18) + 18mn - 12m - 24n - 12$$

$$= \left[\frac{1}{2}\right](27mn - 9m + 36n + 18) + 18mn - 3m - 24n - 12$$

$$=94.5mn-7.5m-6n-3$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

$SK_1(SL(m,n)) = 81mn-31.5m-36n-18$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m)\left[\frac{9}{2}\right]+(3mn-m+4n+2)[9]+(3mn-2m-4n-2)[18]$$

$$=\left[\frac{1}{2}\right](27m)+27mn-9m+36n+18+54mn-36m-72n-36$$

$$=\left[\frac{1}{2}\right](27m)+81mn-45m-36n-18$$

$$=81mn-31.5m-36n-18$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

$SK_2(SL(m,n)) = 108mn-45.5m-143n-71.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m)[3]^2+(3mn-m+4n+2)\left[\frac{9}{2}\right]^2+(3mn-2m-4n-2)[6]^2$$

$$=27m+\left[\frac{1}{4}\right](3mn-m+4n+2)+108mn-72m-144n-72$$

$$=\left[\frac{1}{4}\right](3mn-m+4n+2)+108mn-45m-144n-72$$

$$=108mn-45.5m-143n-71.5$$

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest related to the publication of this article.

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GLOBAL JOURNAL OF APPLIED ENGINEERING MATHEMATICS
Vol. 01 (2019) 14-34
www.knowvel.com

Original Research Article

ON COMPUTATION OF NEW DEGREE-BASED TOPOLOGICAL INDICES OF SILICATE CHAIN GRAPH

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ABSTRACT

The Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2 indices of a graph G was introduced by V. S. Shigehalli and R. R. Kanabur. These topological indices explain the modeling of various physico-chemical, biological and pharmacological properties of organic molecules in chemistry and explains studies of various results on Silicate Chain Graph.

Keywords: Molecular graph, arithmetic-geometric index (AG_1 index), SK index, SK_1 index, SK_2 index, silicate chain graph

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PUBLICATION HISTORY

Received: May 31, 2019
Accepted: June 12, 2019

ARTICLE ID: GJAEM-73

1. INTRODUCTION

In chemical graph theory, we have many different topological index of arbitrary molecular graph *G*. A topological index of a graphs is a member related to a graph which is invariant under graph automorphisms, obviously, every topological index defines a counting polynomial and vice versa [1, 2].

Construction of the Silicate Chain Graph:

SiO_4 tetrahedral are found nearly in all the silicates. Silicates are immensely essential and complicated minerals. We get silicate from metal carbonates with sand or from fusing metal oxides. Silicates behave as the building blocks of the usual rock-forming minerals [3]. Consider a single tetrahedron (i.e., a pyramid having a triangular base). Place oxygen atoms at the four corners of a tetrahedron, and the silicon atom is bonded with equally-spaced atoms of oxygen. The resulting tetrahedron is a silicate tetrahedron, which is shown in figure 1a, and when this tetrahedron join with other tetrahedral joins with other tetrahedral linearly, then a single-row silicate chain is formed, as shown in figure 1b. When two tetrahedral join together corner-to-corner, then each tetrahedron shares its oxygen atom with the other tetrahedron, as shown in figure 1c. After this sharing, these two tetrahedral can be joined with two other tetrahedral, as in figure 1e, were *m* is the number of row lines and *n* is the number of edges in a row line [3].

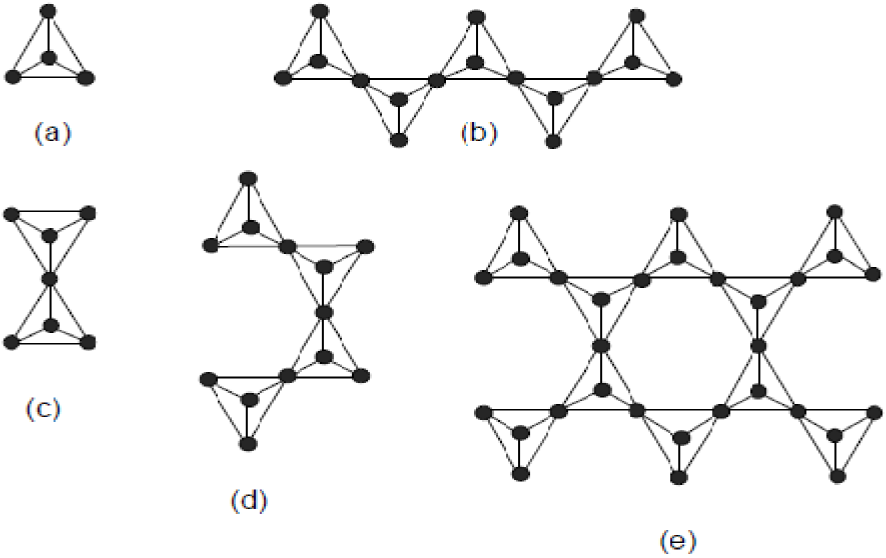

Figure 1. Chain silicate network

2. Survey of Certain Degree-Based Topological Indices

Motivated by previous research on Nanotubes [3-9], here we compute the values of four new topological indices of silicate chain.

Arithmetic-Geometric (*AG_1*) Index: Let *G = (V, E)* be a molecular graph, and $d_G(u)$ is the degree of the vertex *u*, then AG_1 index of *G* is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}} \tag{1}$$

Where, AG_1 index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of *u* and *v*, where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex *u* (or *v*).

***SK* Index:** The *SK* index of a graph *G = (V, E)* is defined as,

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2} \tag{2}$$

Where, $d_G(u)$ and $d_G(v)$ are the degrees of the vertices *u* and *v* in *G*.

***SK_1* Index:** The SK_1 index of a graph *G = (V, E)* is defined as,

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2} \tag{3}$$

Where, $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices *u* and *v* in *G*.

***SK_2* Index:** The SK_2 index of a graph *G = (V, E)* is defined as,

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2 \tag{4}$$

Where, $d_G(u)$ and $d_G(v)$ are the degrees of the vertices *u* and *v* in *G*.

3. RESULTS AND DISCUSSION

In this section, we calculate the closed results for topological indices, which based on vertex degrees of the m^{th} silicate chain. We compute the. The number of edges of the m^{th} chain silicate are 6mn. In the following theorem, the degree-based topological indices for the m^{th} chain silicate is computed.

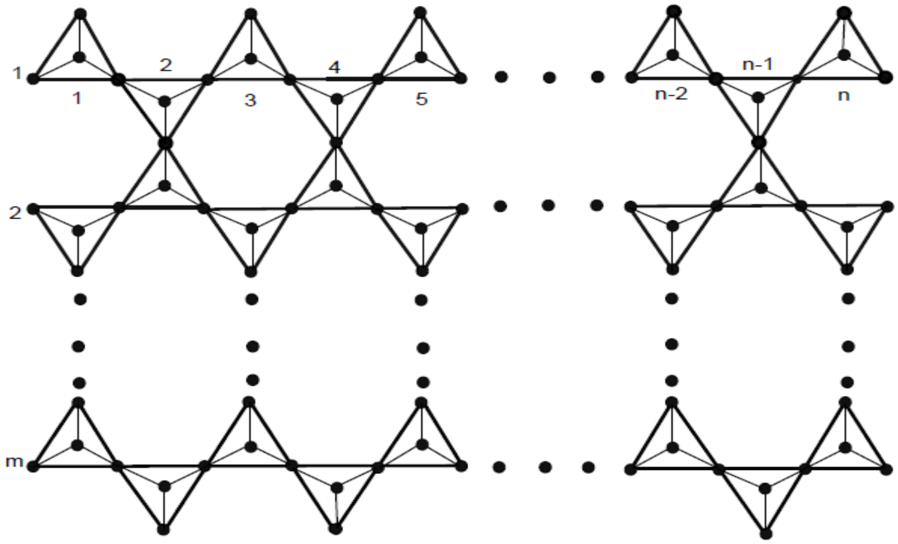

Figure 2. m^{th} chain silicate *(SL(m,n))*

Table 1. Edge partition of silicate chain (SL(m,n)) when m=n based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+2
(3,6)	3mn+3n-4
(6,6)	3mn-6n+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG$_1$) index is equal to

AG$_1$ (SL(m,n)) = $6.18mn + 3m + 21n - 0.242$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.1 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right] + (3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right] + (6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+2)\left[\frac{6}{2\sqrt{9}}\right] + (3mn+3n-4)\left[\frac{9}{2\sqrt{18}}\right] + (3mn-6n+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= 3m+2 + \left[\frac{1}{2\sqrt{18}}\right](27mn+27n-36) + 3mn - 6n + 2$$

$$= 3mn+3m-6n+4 + \left[\frac{1}{2\sqrt{18}}\right](27mn+27n-36)$$

$$= 6.18mn + 3m + 21n - 0.242$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn+9m-22.5n$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.1 we compute the SK index of G which is expressed as

$$SK(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+2)[3]+(3mn+3n-4)\left[\frac{9}{2}\right]+(3mn-6n+2)[6]$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+2)[3]+(3mn+3n-4)\left[\frac{9}{2}\right]+(3mn-6n+2)[6]$$

$$=18mn+9m-36n+18+\frac{1}{2}[27mn-36n-36]$$

$$=31.5mn+9m-22.5n$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $13.5m+9+81mn-81n$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+2)\left[\frac{9}{2}\right]+(3mn+3n-4)[9]+(3mn-6n+2)[18]$$

$$=\frac{1}{2}[27m+18]+27mn+27n-36+54mn-108n+36$$

$$=\frac{1}{2}[27m+18]+81mn-81n$$

$$=13.5m+9+81mn-81n$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $168.75mn+27m-155.25n+9$

Proof: Consider the silicate chain (SL(m,n)), when m=n. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.1 we compute the SK_2 index of G which is expressed as

$$SK_2\,(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$$

$$= (3,3)\left[\frac{3+3}{2}\right]^2 + (3,6)\left[\frac{3+6}{2}\right]^2 + (6,6)\left[\frac{6+6}{2}\right]^2$$

$$= (3m+2)[3]^2 + (3mn+3n-4)\left[\frac{9}{2}\right]^2 + (3mn-6n+2)[6]^2$$

$$= 27m + 18 + \frac{1}{4}[3mn+3n-4] + 108mn - 216n + 72$$

$$= 108mn - 27m - 216n + 90 + \left[\frac{1}{4}\right]\left(27mn + 9m + 18n - 54\right)$$

$$= 168.75mn + 27m - 155.25n + 9$$

Table 2. Edge partition of silicate chain (SL(m,n)) when m<n and m is odd based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	**Number of Edges**
(3,3)	3m+3
(3,6)	3mn+m+2n-5
(6,6)	3mn-2n-4m+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $12.18mn - 7.94m - 3.88n + 0.697$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) + d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right] + (3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right] + (6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+3)\left[\frac{6}{2\sqrt{9}}\right] + (3mn + m + 2n - 5)\left[\frac{9}{2\sqrt{18}}\right] + (3mn - 2n - 4m + 2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn + 9m + 18n - 45) + 3m + 3 + 9mn - 6n - 12m + 6$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn + 9m + 18n - 45) + 9mn - 9m - 6n + 9$$

$$= 12.18mn - 7.94m - 3.88n + 0.697$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn - 1.5m - 12n - 1.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the SK index of G which is expressed as

SK(G)= $\sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+3)[3]+(3mn+m+2n-5)\left[\frac{9}{2}\right]+(3mn-2n-4m+2)[6]$$

$$=18mn-15m-12n+21+\left[\frac{1}{2}\right](27mn+9m+18m-45)$$

$$=31.5mn-1.5m-12n-1.5$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_1$ index is equal to

SK$_1$ (SL(m,n)) = $81mn - 51.5m - 54n + 4.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the SK$_1$ index of G which is expressed as

SK$_1$(G) = $\sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+3)\left[\frac{9}{2}\right]+(3mn+m-2n-5)[9]+(3mn-2n-4m+2)[18]$$

$$=\frac{1}{2}[27m+27]+27mn+9m-18n-45+54mn-36n-72m+36$$

$$=\frac{1}{2}[27m+27]+81mn-65m-54n-9$$

$$=81mn-51.5m-54n+4.5$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_2$ index is equal to

SK$_2$ (SL(m,n)) = $168.75mn - 96.75m - 31.5n + 2.25$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.2 we compute the SK$_2$ index of G which is expressed as

SK$_2$ (G) = $\sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+3)[3]^2+(3mn+m+2n-5)\left[\frac{9}{2}\right]^2+(3mn-2n-4m+2)[6]^2$$

$$=27m+27+\frac{1}{4}[243mn+81m+162n-405]+108mn-72n-144m+72$$

$$=108mn-117m-72n+99+\left[\frac{1}{4}\right](243mn+81m+162n-405)$$

$$=168.75mn-96.75m-31.5n+2.25$$

Table 3. Edge partition of silicate chain (SL(m,n)) when m<n and m is even, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	**Number of Edges**
(3,3)	3m+6
(3,6)	3mn+m+2n-8
(6,6)	3mn-2n-4m+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn-0.06m+0.12n-0.48$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=(3m+6)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+m+2n-8)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2n-4m+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-72)+3mn-m-2n+8$$

$$=6.18mn-0.06m+0.12n-0.48$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn-10.5m-3n-6$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the SK index of G which is expressed as

$$SK(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=\left(3m+3\right)\left[3\right]+(3mn+m+2n-5)\left[\frac{9}{2}\right]+\left(3mn-2n-4m+2\right)\left[6\right]$$

$$=18mn-15m-12n+30+\left[\frac{1}{2}\right]\left(27mn+9m+18m-72\right)$$

$$=31.5mn-10.5m-3n-6$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $8mn-49.5m-18n-9$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the SK_1 index of G which is expressed as

$$SK_1(G)=\sum_{uv\in E(G)}\frac{d_G\left(u\right).d_G\left(v\right)}{2}$$

$$=\left(3,3\right)\left[\frac{3.3}{2}\right]+\left(3,6\right)\left[\frac{3.6}{2}\right]+\left(6,6\right)\left[\frac{6.6}{2}\right]$$

$$=\left(3m+6\right)\left[\frac{9}{2}\right]+(3mn+m-2n-8)\left[9\right]+\left(3mn-2n-4m+2\right)\left[18\right]$$

$$=\left[\frac{1}{2}\right]\left(27m+54\right)+27mn+9m+18n-72+54mn-36n-72m+36$$

$$=\left[\frac{1}{2}\right]\left(27m+54\right)+8mn-63m-18n-36$$

$$=8mn-49.5m-18n-9$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $168.75mn-96.75m-31.5n-36$

Proof: Consider the silicate chain (SL(m,n)), when m<n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.3 we compute the SK_2 index of G which is expressed as

$$SK_2\ (G)=\sum_{u,v\in E(G)}\left(\frac{d_G\left(u\right)+d_G\left(v\right)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+6)[3]^2+(3mn+m+2n-8)\left[\frac{9}{2}\right]^2+(3mn-2n-4m+2)[6]^2$$

$$=27m+54+\left[\frac{1}{4}\right]\left(243mn+81m+162n-648\right)+108mn-72n-144m+72$$

$$=108mn-72n-117m+126+\left[\frac{1}{4}\right]\left(243mn+81m+162n-648\right)$$

$$=168.75mn-96.75m-31.5n-36$$

Table 4. Edge partition of silicate chain (SL(m,n)) when m<n and m & n both are even, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	**Number of Edges**
(3,3)	3m+4
(3,6)	3mn+m+2n-6
(6,6)	3mn-4m-2n+2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+0.06m+0.12n-0.36$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=(3m+4)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+m+2n-6)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-4m-2n+2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-m-2n+6$$

$$=6.18mn+0.06m+0.12n-0.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn-10.5m-3n-3$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=\left(3,3\right)\left[\frac{3+3}{2}\right]+\left(3,6\right)\left[\frac{3+6}{2}\right]+\left(6,6\right)\left[\frac{6+6}{2}\right]$$

$$=\left(3m+4\right)\left[3\right]+(3mn+m+2n-6)\left[\frac{9}{2}\right]+\left(3mn-4m-2n+2\right)\left[6\right]$$

$$=18mn-15m-12n+24+\left[\frac{1}{2}\right]\left(27mn+9m+18n-54\right)$$

$$=31.5mn-10.5m-3n-3$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn-49.5m-18n$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+4)\left[\frac{9}{2}\right]+(3mn+m+2n-6)[9]+(3mn-4m-2n+2)[18]$$

$$=\left[\frac{1}{2}\right](27m+36)+27mn+9m-18n-54+54mn-72m-36n+36$$

$$=\left[\frac{1}{2}\right](27m+36)+81mn-63m-18n-18$$

$$=81mn-49.5m-18n$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $114.75mn-114.75m-67.5n+94.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.4 we compute the SK_2 index of G which is expressed as

$$SK_2\,(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+4)[3]^2+(3mn+m+2n-6)\left[\frac{9}{2}\right]^2+(3mn-4m-2n+2)[6]^2$$

$$=27m+36+\left[\frac{1}{4}\right](27mn+9m+18n-54)+108mn-144m-72n+72$$

$$=108mn-117m-72n+108+\left[\frac{1}{4}\right](27mn+9m+18n-54)$$

$$=114.75mn-114.75m-67.5n+94.5$$

Table 5. Edge partition of silicate chain (SL(m,n)) when m<n and m & n both are odd, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+4
(3,6)	3mn+3m-2
(6,6)	3mn-6m-2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+0.18m-4.12$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+4)\left[\frac{6}{2\sqrt{9}}\right]+(3mn+3m-2)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-6m-2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= (3m+4)[1]+\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-6m-2$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-3m-2$$

$$= 6.18mn+0.18m-4.12$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn+4.5m-9$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$= (3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$= (3m+4)[3]+(3mn+3m-2)\left[\frac{9}{2}\right]+(3mn-6m-2)[6]$$

$$= \quad 9m+12+\left[\frac{1}{2}\right](27mn+27m-18)+18mn-36m-12$$

$$= \left[\frac{1}{2}\right](27mn+27m-18)+18mn-27m$$

$= 31.5mn + 4.5m - 9$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn - 67.5m - 36$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$= (3,3)\left[\frac{3.3}{2}\right] + (3,6)\left[\frac{3.6}{2}\right] + (6,6)\left[\frac{6.6}{2}\right]$$

$$= (3m+4)\left[\frac{9}{2}\right] + (3mn + m + 2n - 6)[9] + (3mn - 4m - 2n + 2)[18]$$

$$= \left[\frac{1}{2}\right](27m + 36) + 27mn + 9m - 18n - 54 + 54mn - 72m - 36n + 36$$

$$= \left[\frac{1}{2}\right](27m + 36) + 81mn - 63m - 18n - 18$$

$$= 81mn - 67.5m - 36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $168.75mn - 148.5m - 76.5$

Proof: Consider the silicate chain (SL(m,n)), when m<n, m and n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.5 we compute the SK_2 index of G which is expressed as

$$SK_2\ (G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2$$

$$= (3,3)\left[\frac{3+3}{2}\right]^2 + (3,6)\left[\frac{3+6}{2}\right]^2 + (6,6)\left[\frac{6+6}{2}\right]^2$$

$$= (3m+4)[3]^2 + (3mn + m + 2n - 6)\left[\frac{9}{2}\right]^2 + (3mn - 4m - 2n + 2)[6]^2$$

$$= 27m + 36 + \left[\frac{1}{4}\right](27mn + 9m + 18n - 54) + 108mn - 144m - 72n + 72$$

$$= 108mn - 117m - 72n + 108 + \left[\frac{1}{4}\right](27mn + 9m + 18n - 54)$$

$$= 168.75mn - 148.5m - 76.5$$

Table 6. Edge partition of silicate chain (SL(m,n)) when m>n and m is odd, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+1
(3,6)	3mn-m+4n-1
(6,6)	3mn-2m-4n

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn-1.94m+2.12n-7.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=\left(3m+1\right)\left[\frac{6}{2\sqrt{9}}\right]+(3mn-m+4n-1)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2m-4n)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=(3m+1)[1]+\left[\frac{1}{2\sqrt{18}}\right](27mn-m+4n-1)+3mn-6m-2$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn-3m-1$$

$$=6.18mn-1.94m+2.12n-7.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $19.5mn-3.5m-22n+2.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m+1)[3]+(3mn-m+4n-1)\left[\frac{9}{2}\right]+(3mn-2m-4n)[6]$$

$$= 9m+3+\left[\frac{1}{2}\right](3mn-m+4n-1)+18mn-12m-24n$$

$$=\left[\frac{1}{2}\right](3mn-m+4n-1)+18mn-3m-24n+3$$

$$=19.5mn-3.5m-22n+2.5$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_1$ index is equal to

SK$_1$ (SL(m,n)) = $81mn-31.5m-36n+9$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the SK$_1$ index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+1)\left[\frac{9}{2}\right]+(3mn-m+4n-1)[9]+(3mn-2m-4n)[18]$$

$$=\left[\frac{1}{2}\right](27m+36)+27mn-9m+36n-9+54mn-36m-72n$$

$$=\left[\frac{1}{2}\right](27m+36)+81mn-45m-36n-9$$

$$=81mn-31.5m-36n+9$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_2$ index is equal to

SK$_2$ (SL(m,n)) = $87.75mn-42.75m-139.5n-4.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.6 we compute the SK$_2$ index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+1)[3]^2+(3mn-m+4n-1)\left[\frac{9}{2}\right]^2+(3mn-2m-4n)[6]^2$$

$$=27m+9+\left[\frac{1}{4}\right](27mn+9m+18n-54)+108mn-72m-144n$$

$$=108mn-45m-144n+9+\left[\frac{1}{4}\right](27mn+9m+18n-54)$$

$$=87.75mn-42.75m-139.5n-4.5$$

Table 7. Edge partition of silicate chain (SL(m,n)) when m>n and m is even, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	Number of Edges
(3,3)	3m+4
(3,6)	3mn-m+4n-4
(6,6)	3mn-2m-4n

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+2.060m-1.88n-2.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m+4)\left[\frac{6}{2\sqrt{9}}\right]+(3mn-m+4n-4)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2m-4n)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= (3m+4)[1]+\left[\frac{1}{2\sqrt{18}}\right](3mn-m+4n-4)+3mn-2m-4n$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn+m-4n+4$$

$$= 6.18mn+2.060m-1.88n-2.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $31.5mn-7.5m-6n-6$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$= (3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$= (3m+4)[3]+(3mn-m+4n-4)\left[\frac{9}{2}\right]+(3mn-2m-4n)[6]$$

$$= \quad 9m+12+\left[\frac{1}{2}\right](27mn-9m+36n-36)+18mn-12m-24n$$

$$= \left[\frac{1}{2}\right](27mn-9m+36n-36)+18mn-3m-24n+12$$

$$=31.5mn-7.5m-6n-6$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn-31.5m+36n-90$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m+4)\left[\frac{9}{2}\right]+(3mn-m+4n-4)[9]+(3mn-2m-4n)[18]$$

$$=\left[\frac{1}{2}\right](27m+36)+27mn-9m+36n-36+54mn-36m-72$$

$$=\left[\frac{1}{2}\right](27m+36)+81mn-45m+36n-108$$

$$=81mn-31.5m+36n-90$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $114.75mn-42.75m-139.5n+22.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m is even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.7 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m+4)[3]^2+(3mn-m+4n-4)\left[\frac{9}{2}\right]^2+(3mn-2m-4n)[6]^2$$

$$=27m+36+\left[\frac{1}{4}\right](3mn-m+4n-4)+108mn-72m-144n$$

$$=108mn-45m-144n+36+\left[\frac{1}{4}\right](27mn+9m+18n-54)$$

$$=114.75mn-42.75m-139.5n+22.5$$

Table 8. Edge partition of silicate chain (SL(m,n)) when m>n and m & n both are even, based on the degrees of the end vertices of each edge.

(d_u,d_v) where $uv \in E(G)$	Number of Edges
(3,3)	3m
(3,6)	3mn-m+4n+2
(6,6)	3mn-2m-4n-2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn + 2.060m - 1.88n - 8.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$= (3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right] + (3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right] + (6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$= (3m)\left[\frac{6}{2\sqrt{9}}\right] + (3mn - m + 4n + 2)\left[\frac{9}{2\sqrt{18}}\right] + (3mn - 2m - 4n - 2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$= (3m)[1] + \left[\frac{1}{2\sqrt{18}}\right](3mn - m + 4n + 2) + 3mn - 2m - 4n - 2$$

$$= \left[\frac{1}{2\sqrt{18}}\right](27mn + 9m + 18n - 54) + 3mn + m - 4n - 2$$

$$= 6.18mn + 2.060m - 1.88n - 8.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK (SL(m,n)) = $94.5mn - 7.5m - 6n - 3$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the SK index of G which is expressed as

$$SK(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$= (3,3)\left[\frac{3+3}{2}\right] + (3,6)\left[\frac{3+6}{2}\right] + (6,6)\left[\frac{6+6}{2}\right]$$

$$= (3m)[3] + (3mn - m + 4n + 2)\left[\frac{9}{2}\right] + (3mn - 2m - 4n - 2)[6]$$

$$= \quad 9m + \left[\frac{1}{2}\right](27mn - 9m + 36n + 18) + 18mn - 12m - 24n - 12$$

$$= \left[\frac{1}{2}\right](27mn - 9m + 36n + 18) + 18mn - 3m - 24n - 12$$

$$= 94.5mn - 7.5m - 6n - 3$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_1 index is equal to

SK_1 (SL(m,n)) = $81mn - 31.5m - 36n - 18$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$= (3,3)\left[\frac{3.3}{2}\right] + (3,6)\left[\frac{3.6}{2}\right] + (6,6)\left[\frac{6.6}{2}\right]$$

$$= (3m)\left[\frac{9}{2}\right] + (3mn - m + 4n + 2)[9] + (3mn - 2m - 4n - 2)[18]$$

$$= \left[\frac{1}{2}\right](27m) + 27mn - 9m + 36n + 18 + 54mn - 36m - 72n - 36$$

$$= \left[\frac{1}{2}\right](27m) + 81mn - 45m - 36n - 18$$

$$= 81mn - 31.5m - 36n - 18$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK_2 index is equal to

SK_2 (SL(m,n)) = $108mn - 45.5m - 143n - 71.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are even. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.8 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2$$

$$= (3,3)\left[\frac{3+3}{2}\right]^2 + (3,6)\left[\frac{3+6}{2}\right]^2 + (6,6)\left[\frac{6+6}{2}\right]^2$$

$$= (3m)[3]^2 + (3mn - m + 4n + 2)\left[\frac{9}{2}\right]^2 + (3mn - 2m - 4n - 2)[6]^2$$

$$= 27m + \left[\frac{1}{4}\right](3mn - m + 4n + 2) + 108mn - 72m - 144n - 72$$

$$= \left[\frac{1}{4}\right](3mn - m + 4n + 2) + 108mn - 45m - 144n - 72$$

$$= 108mn - 45.5m - 143n - 71.5$$

Table 9. Edge partition of silicate chain (SL(m,n)) when m>n and m & n both are odd, based on the degrees of the end vertices of each edge

(d_u,d_v) where uv ∈ E(G)	**Number of Edges**
(3,3)	3m
(3,6)	3mn-m+4n+2
(6,6)	3mn-2m-4n-2

Theorem: Consider the silicate chain (SL(m,n)), then its Arithmetic-Geometric (AG_1) index is equal to

AG_1 (SL(m,n)) = $6.18mn+2.060m-1.88n-8.36$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the Arithmetic-Geometric index of G which is expressed as

$$AG_1(G) = \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)+d_G(v)}}$$

$$=(3,3)\left[\frac{3+3}{2\sqrt{3.3}}\right]+(3,6)\left[\frac{3+6}{2\sqrt{3.6}}\right]+(6,6)\left[\frac{6+6}{2\sqrt{6.6}}\right]$$

$$=(3m)\left[\frac{6}{2\sqrt{9}}\right]+(3mn-m+4n+2)\left[\frac{9}{2\sqrt{18}}\right]+(3mn-2m-4n-2)\left[\frac{12}{2\sqrt{36}}\right]$$

$$=(3m)[1]+\left[\frac{1}{2\sqrt{18}}\right](3mn-m+4n+2)+3mn-2m-4n-2$$

$$=\left[\frac{1}{2\sqrt{18}}\right](27mn+9m+18n-54)+3mn+m-4n-2$$

$$=6.18mn+2.060m-1.88n-8.36$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK index is equal to

SK(SL(m,n)) = $94.5mn-7.5m-6n-3$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the SK index of G which is expressed as

$$SK(G)= \sum_{uv\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$=(3,3)\left[\frac{3+3}{2}\right]+(3,6)\left[\frac{3+6}{2}\right]+(6,6)\left[\frac{6+6}{2}\right]$$

$$=(3m)[3]+(3mn-m+4n+2)\left[\frac{9}{2}\right]+(3mn-2m-4n-2)[6]$$

$$= \quad 9m+\left[\frac{1}{2}\right](27mn-9m+36n+18)+18mn-12m-24n-12$$

$$=\left[\frac{1}{2}\right](27mn-9m+36n+18)+18mn-3m-24n-12$$

$=94.5mn-7.5m-6n-3$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_1$ index is equal to

SK$_1$(SL(m,n)) = $81mn-31.5m-36n-18$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the SK$_1$ index of G which is expressed as

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$=(3,3)\left[\frac{3.3}{2}\right]+(3,6)\left[\frac{3.6}{2}\right]+(6,6)\left[\frac{6.6}{2}\right]$$

$$=(3m)\left[\frac{9}{2}\right]+(3mn-m+4n+2)[9]+(3mn-2m-4n-2)[18]$$

$$=\left[\frac{1}{2}\right](27m)+27mn-9m+36n+18+54mn-36m-72n-36$$

$$=\left[\frac{1}{2}\right](27m)+81mn-45m-36n-18$$

$$=81mn-31.5m-36n-18$$

Theorem: Consider the silicate chain (SL(m,n)), then its SK$_2$ index is equal to

SK$_2$ (SL(m,n)) = $108mn-45.5m-143n-71.5$

Proof: Consider the silicate chain (SL(m,n)), when m>n and m & n both are odd. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in table.9 we compute the SK$_2$ index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$=(3,3)\left[\frac{3+3}{2}\right]^2+(3,6)\left[\frac{3+6}{2}\right]^2+(6,6)\left[\frac{6+6}{2}\right]^2$$

$$=(3m)[3]^2+(3mn-m+4n+2)\left[\frac{9}{2}\right]^2+(3mn-2m-4n-2)[6]^2$$

$$=27m+\left[\frac{1}{4}\right](3mn-m+4n+2)+108mn-72m-144n-72$$

$$=\left[\frac{1}{4}\right](3mn-m+4n+2)+108mn-45m-144n-72$$

$$=108mn-45.5m-143n-71.5$$

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest related to the publication of this article.

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ISSN: 0976-3031

Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(D), pp. 36499-36503, December, 2019

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOASSAY OF HEAVY METALS POLLUTION IN ROADSIDE ENVIRONMENT: BIOINDICATORS

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4934

ARTICLE INFO

Article History:

Received 10th September, 2019
Received in revised form 2nd October, 2019
Accepted 26th November, 2019
Published online 28th December, 2019

Key Words:

Phytoassay, Bio indicators, Heavy metals, Food chain, anthropogenic activities, phytotool.

ABSTRACT

The Lead, Copper, Zinc Manganese, Nickel, Chromium and Cadmium contents in roadside grass, *Setaria verticellata* (L) P. Beaur (Family-Poaceae), *Ficus bengalensis* L. (Family- Moraceae) and soil from six sampling sites on state highway with heavy traffic loads passing through the city of Jamkhandi (Karnataka) were determined by atomic absorption spectrophotometer Results showed that soil, grass and *Ficus* contained elevated levels of the metals examined. Primarily it was found that the contamination occurs mainly by arial deposition of dust and the vehicular emissions. Apparently it was found that both soil and test plants can be utilized to reflect the roadside environment. The increased circulation of toxic metals in inevitable build-up of xenobiotic in food chain. The variation in heavy metal concentrations is due to changes in traffic density and anthropogenic activities. It is concluded that *Ficus* and *setaria* (grass) can be used as phytotool to monitor heavy metal pollution in roadside plants.

INTRODUCTION

Plants are important indicators of heavy metals environmental pollution (1). Environmental heavy metal pollution is mainly due to anthropogenic origin and results from the activities such as fossil fuels, vehicular emission, industrial emissions, landfill leachates, fertilizers, sewage and municipal wastes (2,3,4,5) Various plants have been used as bio indicators to assess the impact of a pollution source on the vicinity which is due to high metal accumulation of plants (6,7) worked on the basic criteria for the selection of species as a bio indicators. Now a days toxic effects of heavy metal are burning issue and been studied by many researchers (8,9). Entrance of heavy metals may occur in human and animal food chain as a results of their uptake by edible plants grown in an contaminated soil (10). The toxic and hazardous effects of some heavy metals on human health are very significant and may cause many fatal diseases. Lead (Pb) is one of the heavy metal that is responsible for anaemia, neurological disorder, hyperactivity and changes in blood enzymes in the human body (11) Cadmium and Zinc are important toxic metals & long time exposure of which causes renal pulmonary, hepatic, skeletal reproductive and many other carcinogenic effects (12,13) Many studies have been made on Pb, little attention has been focused on the contamination of other trace metals on the roadside environment. Metal such as iron, Copper, Zinc, Chromium (Vl), Cadmium, Manganese and Nickel are the essential components of many alloys, pipes, wires and tyres in motor vehicles and are released into the roadside environment as a result of mechanical abrasion Medicinal plants of Apocynaceae growing along the roadside have been employed as a phytotool to monitor toxic levels of heavy metals (14). The determination of heavy metal accumulation in roadside soil may be an index of the environmental pollution of Jamkhandi along the state highway towards Rabakavi & Banahatti. Keeping this view, the research was conducted to know the heavy metal accumulation of roadside soil, grass and *ficus* of the research area.

MATERIALS AND METHODS

Jamkhandi is the city of northern region of Karnataka (India) at longitude 16^0 30′ 6″ N and latitude 75^0 16′ 17″. It is well connected with Bagalkot and Vijayapur district of Karnataka state. The city and its surrounding places are suffered from high traffic density caused by vehicles. The grass (*Setaria*) and *Ficus* and soil were collected during summer 2018, which were three meters away from the state highway (Fig1 and table 1) passing from Jamkhandi to Rabhakavi Banhatti. Grass and ficus samples were collected from each site at three random spots that were spaced approximately at 1 m interval. The

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leaves were clipped with stainless steel scissors. All the samples of each site were then combined to give composite samples of about 300-500 g.

The leaves of grass (*Setaria)* and *Ficus* samples were dried at 80^0C for 48hr fine by powdered and sieved through 0.2mm sieve. One gram sample was digested using Gerhardt digestion unit using mixed acid digestion method. The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made upto 100ml.

Similarly, soil samples were dried, powdered and sieved through 0.2mm sieve. One gram of sample was digested Gerhardt digestion unit according to Allen *et al*. method (mixed acid digestion method). The resulting extracts were diluted and filtered through Whattman No 41 paper and made upto 100ml using double distilled water and analysed for heavy metal viz: Pb (Lead), Cd (Cadmium), Cu (Copper), Zn (Zinc), Mn (Manganese), Ni (Nickel) and Cr (Chromium) with GBC-932 plus Atomic Absorption Spectrometer (AAS) (Australia) with an air/ acetylene flame and metal hollow cathode lamps. Respective wavelengths were used for the estimation of solutions for heavy metals were purchased from Siscochemical Laboratory Bombay (1000 mg/L) for Cd 228.8 nm, Pb 217.0 nm, Ni 232.0 nm, Cu 324.7 nm, Zn 213.9 nm, Mn 279.5 nm and Cr 221.8 nm filters have been used for the estimation using AAS. The working standards were prepared by serial dilution of standard stock solutions and were for the calibration of the instrument.

RESULTS AND DISCUSSION

Environmental pollution with toxic metals has been dramatically increased since the increasing of vehicular exhausts (16). The pollution by heavy metals Viz, Pb, Cd, Cr, Ni, Mn, Zn etc, it is problem of concern (17). It is necessary to determine the kinds of environmental pollution and how for these exhibit and act as an efficient bio indicator in reducing the degree of pollution in the environment. The samples were collected along the state highway between Jamkhandi to Rabhakavi Banhatti for the estimation of heavy metals (Table.1).

The range arithmetic mean of heavy metal concentration of soil, ficus and grass samples of state highway and control sites are presented in Table 4. Correlation co-efficient of heavy metals in roadside soil, grass and ficus plant samples are given in the Table 3 and 4.

Lead is a poisonous metal in human it is directly absorbed into the blood stream and is stored in soft tissues, bones and teeth (18). The main source of Pb is exhaust fume**s** of automobiles, chimneys of factories, road side vehicles pollution (19). The results of our analysis shows that there are significant difference for lead between sampling sites in control the polluted area. Results shows that soil tends to accumulate more Pb than grass and the highest Pb level found in the roadside soil was 140.10µg /gm while for Ficus 28.94µg /gm and for the grass it was 29.25µg /gm. The mean soil Pb level is 94.98µg /gm indicated considerable contamination of the metal in the roadside environment, where as local soil control has baseline level of 70.50µg/gm Pb. The lead deposited on the vegetation reaches the soil by rain water from the surface and also by the death and decomposition of the plant. When incorporated in the soil Pb is of very low mobility. Hence, once contaminated a soil is liable to retain polluted with lead. The lead deposited in soil and vegetation can also cause enhanced levels of lead in soil (20,21).

Roadside soil gave higher Cu concentration due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of car derived from engine wear brushing and bearing metals (22) Copper is essential element but higher concentration intake leads to severe mucosal irritation, wide spread capillary damage, renal and hepatic damage (23). The mean Cu level in road soil (48.98µg/gm) indicated considerable concentration of metal however, it was found to be much higher than the grass(4.70µg/gm) and ficus (4.86µg/gm).

The source of Zn in relation to automobile traffic is wearing of break lining, loses of oil and cooling liquid (24). Excess amount of Zn can cause in impairment of growth and reproduction. Excess Zn in the body bound in various transcription regions such as polymerase enzyme (25). Similar results were also reported by (26).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process, thus the plants can easily absorb Cd from the soil. The Cd in excess reported that the disruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of cadmium toxicity (27). Our analysis for Cd in the roadside plants and soil showed that there significant differences between polluted and control area. Cadmium level in roadside soil averaged about 2.0µgm. The mean Cd in ficus is 1.39 µg/gm and in grass 1.57 µg/gm. The results are in confirmation with the findings of Ho and Tai, (28).

Manganese is micronutrient essential for physiological functions but higher concentrations is toxic causing neuropsychiatic disorders (29). The soil grass and ficus contained much higher levels of Mn than other metals examined. The higher content may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil.The roadside soil, grass and ficus had average 1527.2 µg/gm, 56.0 µg/gm and 56.09 µg/gm of Mn respectively.

Chromium is considerable as a serious pollutant due to wide industrial use (30). Chromium can cause nose irritation, respiratory damages and also liver and kidney and also it brings about alternation of genetical material (31) & Chromium level was very high in roadside soil 314.51 µg/gm against control value of 111.21 µg/gm. In grass it was 4.89 µg/gm and in ficus it was found to be 4.61 µg/gm against the control (Zero).

Nickel has been considerable to be as essential trace element for human and animal health (32). Due to bioaccumulation it shows skin irritation, damage to the lungs and nervous system (33). Ni level was considerable and was in roadside soil 85.2 µg/gm against control value 68.25 µg/gm. In grass it was 10.49 µg/gm and in ficus it was found to be 9.10 µg/gm against control 6.51 µg/gm.

Simple linear regression between the metals Viz, Pb, Cu, Ni, Mn, Zn, Cr and Cd present in the soil, grass and Ficus were calculated and are given in the tables 2&3. According to simple linear regression between the metal levels in roadside soil, grass and ficus were found in Zn, Cd, and Ni are

significant at 5% level (P>0.05). It may be indicating the bio concentration of these metals in the ficus, grass in addition to aerial deposition, This may attributed to the favourable root environment (34) i.e, Soil conditions might have favoured their absorption (35).

Correlations in case of chromium, nickel, manganese and copper contents between soil, grass and ficus were low due to low bioavailability of these metals owingto unfavourable root environment. Whatever excess content of these metals found in grass and ficus was presumed due to aerial deposition contributed by vehicular and other anthropogenic activities.

The elevated levels of heavy metals in roadside soil, ficus and grass are an indication of airborne pollutants of roadside environment of the urban area of Jamkhandi and surroundings. Soils have high retention capacity for the heavy metals are due to their cat ion exchange capacity (CEC), Complex organic substances, oxides and carbonates. Similar observations were also made by Tambavani and vathana (36) in *Azadirect indica* in madhurai city of southern region of Tamil Nadu.

The order increment of heavy metals in roadside is as follows:
In soil Mn > Cr > Zn > Pb > Ni > Cu > Cd
In grass Mn > Zn > Pb > Ni > Cr > Cu > Cd
In ficus Mn > Zn > Pb > Ni > Cu > Cr > Cd.

In soil the lesser mobility of metals and its accumulation on a long term basis , leads to overall higher concentration level of metals; where as in roadside ficus and grass, represents more recent accumulation due to new growth the substance followed by abscission of old parts and meteorological influences. Thus, the study of metal concentration of roadside soil, grass and ficus bordering the state highway, for livestock feeding may result in deleterious consequences from nutritional and veterinary hygienic point of view. The penetration of heavy metals into food chains due to vehicular emissions may cause a long range ecological and health hazards.

Acknowledgements

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi, India, and PG Department Botany, Karnatak University Dharwad (India) for providing necessary facilities to carry out research work.

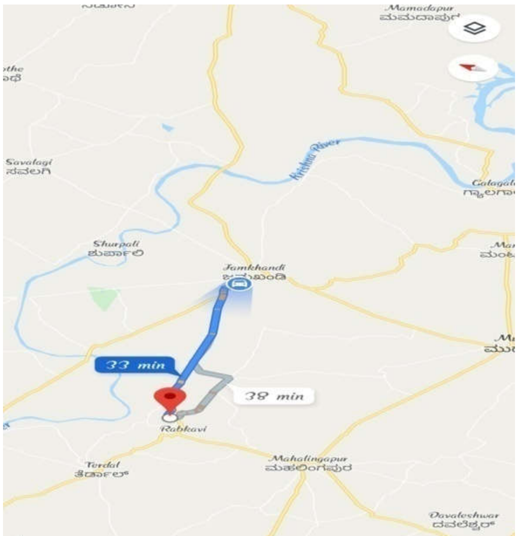

Fig 1 Map showing the state highway from Jamkhandi to Rabakavi-Banhatti.

Table 1 Sampling station along the state- highway from Jamkhandi to Rabakavi-Banhatti

Station No.	Sampling station	Nature of station
Control	Jamkhandi (City)	Unpolluted city vehicular movement is negligible
1	Hunnur	Unpolluted area with less distribution. Vehicular movement is high agricultural fields on either side of the road.
2	Madhurakhandi	Brick factories around and vehicular traffic is high
3	Bandigani cross	Vehicular movement is high with high vehicular traffic.
4	Yallatti	Vehicular movement is high with high vehicular Traffic.
5	Asangi (Near DEMP)	Brick factories around near to Rabkavi-Banhatti city with high vehicular traffic.
6	Rabakavi-Banhatti	Vehicular movement is high with high vehicular traffic.

Table 2 Metal accumulation profile in ficus, grass and soil

Sr. No.	Heavy metals	Control group (µg g^{-1}dry wt)	Roadside Ficus (µg g^{-1} dry wt)		Roadside grass (µg g^{-1} dry wt)		Control (µg g^{-1}dry wt)	Roadside soil (µg g^{-1} dry wt)	
			Range	Mean ± SE	Range	Mean ± SE		Range	Mean ± SE
1	Lead	17.96	20.32-28.94	23.41±1.81	20.41-29.25	23.73±1.84	70.50	82.90-140.1	94.98±8.64
2	Copper	2.10	3.91-4.98	4.70±0.34	3.92-5.56	4.86±0.34	39.95	38.74-58.21	48.98±3.49
3	Zinc	15.91	24.21-35.7	32.54±3.81	24.20-34.5	32.87±3.10	29.89	32.29-389-51	187.9±53.25
4	Cadmium	0.81	1.11-1.74	1.39±0.07	1.20-1.82	1.57±0.081	2.13	1.75-2.89	2.0±0.18
5	Manganese	11.91	24.08-71.18	56.09±3.29	28.89-72.22	56.61±7.32	1251.4	1257.8-2058.5	1527.2±26.1
6	Chromium	ND	1.20-8.1	4.61±2.20	1.30-8.91	4.89±2.21	111.21	131.4-954.2	314.51±2.41
7	Nickel	6.51	8.1-148	9.10±1.40	8.7-15.1	10.49±1.41	68.25	70.49-108.4	85.2±5.74

*ND- Not detectable

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus. Significant at 5% P< 0.05)

Sl.No.	Metal	r-Value
1	Lead	0.638*
2	Copper	0.485
3	Zinc	0.824*
4	Cadmium	0.742*
5	Manganese	15.17
6	Nickel	6.61
7	Chromium	0.215

r = 0.60 and above have significant correlation

Table 4 Correlation of heavy metals in roadside soil and grass (Significant at 5% level (P< 0.05).

Sl. No.	Metal	r-Value
1	Lead	0.625*
2	Copper	0.499
3	Zinc	0.818*
4	Cadmium	0.699*
5	Manganese	0.524
6	Nickel	0.334
7	Chromium	0.214

r = 0.60 and above have significant correlation

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How to cite this article:

Rolli N.M *et al*.2019, Phytoassay of Heavy Metals Pollution in Roadside Environment: Bioindicators. *Int J Recent Sci Res.* 10(12), pp. 36499-36503. DOI: http://dx.doi.org/10.24327/ijrsr.2020.1012.4934

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(D), pp. 36499-36503, December, 2019

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOASSAY OF HEAVY METALS POLLUTION IN ROADSIDE ENVIRONMENT: BIOINDICATORS

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4934

ARTICLE INFO

Article History:

Received 10th September, 2019
Received in revised form 2nd October, 2019
Accepted 26th November, 2019
Published online 28th December, 2019

Key Words:

Phytoassay, Bio indicators, Heavy metals, Food chain, anthropogenic activities, phytotool.

ABSTRACT

The Lead, Copper, Zinc Manganese, Nickel, Chromium and Cadmium contents in roadside grass, *Setaria verticellata* (L) P. Beaur (Family-Poaceae), *Ficus bengalensis* L. (Family- Moraceae) and soil from six sampling sites on state highway with heavy traffic loads passing through the city of Jamkhandi (Karnataka) were determined by atomic absorption spectrophotometer Results showed that soil, grass and *Ficus* contained elevated levels of the metals examined. Primarily it was found that the contamination occurs mainly by arial deposition of dust and the vehicular emissions. Apparently it was found that both soil and test plants can be utilized to reflect the roadside environment. The increased circulation of toxic metals in inevitable build-up of xenobiotic in food chain. The variation in heavy metal concentrations is due to changes in traffic density and anthropogenic activities. It is concluded that *Ficus* and *setaria* (grass) can be used as phytotool to monitor heavy metal pollution in roadside plants.

INTRODUCTION

Plants are important indicators of heavy metals environmental pollution (1). Environmental heavy metal pollution is mainly due to anthropogenic origin and results from the activities such as fossil fuels, vehicular emission, industrial emissions, landfill leachates, fertilizers, sewage and municipal wastes (2,3,4,5) Various plants have been used as bio indicators to assess the impact of a pollution source on the vicinity which is due to high metal accumulation of plants (6,7) worked on the basic criteria for the selection of species as a bio indicators. Now a days toxic effects of heavy metal are burning issue and been studied by many researchers (8,9). Entrance of heavy metals may occur in human and animal food chain as a results of their uptake by edible plants grown in an contaminated soil (10). The toxic and hazardous effects of some heavy metals on human health are very significant and may cause many fatal diseases. Lead (Pb) is one of the heavy metal that is responsible for anaemia, neurological disorder, hyperactivity and changes in blood enzymes in the human body (11) Cadmium and Zinc are important toxic metals & long time exposure of which causes renal pulmonary, hepatic, skeletal reproductive and many other carcinogenic effects (12,13) Many studies have been made on Pb, little attention has been focused on the contamination of other trace metals on the roadside environment. Metal such as iron, Copper, Zinc, Chromium (Vl), Cadmium, Manganese and Nickel are the essential components of many alloys, pipes, wires and tyres in motor vehicles and are released into the roadside environment as a result of mechanical abrasion Medicinal plants of Apocynaceae growing along the roadside have been employed as a phytotool to monitor toxic levels of heavy metals (14). The determination of heavy metal accumulation in roadside soil may be an index of the environmental pollution of Jamkhandi along the state highway towards Rabakavi & Banahatti. Keeping this view, the research was conducted to know the heavy metal accumulation of roadside soil, grass and *ficus* of the research area.

MATERIALS AND METHODS

Jamkhandi is the city of northern region of Karnataka (India) at longitude 16^0 30′ 6″ N and latitude 75^0 16′ 17″. It is well connected with Bagalkot and Vijayapur district of Karnataka state. The city and its surrounding places are suffered from high traffic density caused by vehicles. The grass (*Setaria*) and *Ficus* and soil were collected during summer 2018, which were three meters away from the state highway (Fig1 and table 1) passing from Jamkhandi to Rabhakavi Banhatti. Grass and ficus samples were collected from each site at three random spots that were spaced approximately at 1 m interval. The

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leaves were clipped with stainless steel scissors. All the samples of each site were then combined to give composite samples of about 300-500 g.

The leaves of grass (*Setaria)* and *Ficus* samples were dried at 80^0C for 48hr fine by powdered and sieved through 0.2mm sieve. One gram sample was digested using Gerhardt digestion unit using mixed acid digestion method. The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made upto 100ml.

Similarly, soil samples were dried, powdered and sieved through 0.2mm sieve. One gram of sample was digested Gerhardt digestion unit according to Allen *et al*. method (mixed acid digestion method). The resulting extracts were diluted and filtered through Whattman No 41 paper and made upto 100ml using double distilled water and analysed for heavy metal viz: Pb (Lead), Cd (Cadmium), Cu (Copper), Zn (Zinc), Mn (Manganese), Ni (Nickel) and Cr (Chromium) with GBC-932 plus Atomic Absorption Spectrometer (AAS) (Australia) with an air/ acetylene flame and metal hollow cathode lamps. Respective wavelengths were used for the estimation of solutions for heavy metals were purchased from Siscochemical Laboratory Bombay (1000 mg/L) for Cd 228.8 nm, Pb 217.0 nm, Ni 232.0 nm, Cu 324.7 nm, Zn 213.9 nm, Mn 279.5 nm and Cr 221.8 nm filters have been used for the estimation using AAS. The working standards were prepared by serial dilution of standard stock solutions and were for the calibration of the instrument.

RESULTS AND DISCUSSION

Environmental pollution with toxic metals has been dramatically increased since the increasing of vehicular exhausts (16). The pollution by heavy metals Viz, Pb, Cd, Cr, Ni, Mn, Zn etc, it is problem of concern (17). It is necessary to determine the kinds of environmental pollution and how for these exhibit and act as an efficient bio indicator in reducing the degree of pollution in the environment. The samples were collected along the state highway between Jamkhandi to Rabhakavi Banhatti for the estimation of heavy metals (Table.1).

The range arithmetic mean of heavy metal concentration of soil, ficus and grass samples of state highway and control sites are presented in Table 4. Correlation co-efficient of heavy metals in roadside soil, grass and ficus plant samples are given in the Table 3 and 4.

Lead is a poisonous metal in human it is directly absorbed into the blood stream and is stored in soft tissues, bones and teeth (18). The main source of Pb is exhaust fume**s** of automobiles, chimneys of factories, road side vehicles pollution (19). The results of our analysis shows that there are significant difference for lead between sampling sites in control the polluted area. Results shows that soil tends to accumulate more Pb than grass and the highest Pb level found in the roadside soil was 140.10µg /gm while for Ficus 28.94µg /gm and for the grass it was 29.25µg /gm. The mean soil Pb level is 94.98µg /gm indicated considerable contamination of the metal in the roadside environment, where as local soil control has baseline level of 70.50µg/gm Pb. The lead deposited on the vegetation reaches the soil by rain water from the surface and also by the death and decomposition of the plant. When incorporated in the soil Pb is of very low mobility. Hence, once contaminated a soil is liable to retain polluted with lead. The lead deposited in soil and vegetation can also cause enhanced levels of lead in soil (20,21).

Roadside soil gave higher Cu concentration due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of car derived from engine wear brushing and bearing metals (22) Copper is essential element but higher concentration intake leads to severe mucosal irritation, wide spread capillary damage, renal and hepatic damage (23). The mean Cu level in road soil (48.98µg/gm) indicated considerable concentration of metal however, it was found to be much higher than the grass(4.70µg/gm) and ficus (4.86µg/gm).

The source of Zn in relation to automobile traffic is wearing of break lining, loses of oil and cooling liquid (24). Excess amount of Zn can cause in impairment of growth and reproduction. Excess Zn in the body bound in various transcription regions such as polymerase enzyme (25). Similar results were also reported by (26).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process, thus the plants can easily absorb Cd from the soil. The Cd in excess reported that the disruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of cadmium toxicity (27). Our analysis for Cd in the roadside plants and soil showed that there significant differences between polluted and control area. Cadmium level in roadside soil averaged about 2.0µgm. The mean Cd in ficus is 1.39 µg/gm and in grass 1.57 µg/gm. The results are in confirmation with the findings of Ho and Tai, (28).

Manganese is micronutrient essential for physiological functions but higher concentrations is toxic causing neuropsychiatic disorders (29). The soil grass and ficus contained much higher levels of Mn than other metals examined. The higher content may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil.The roadside soil, grass and ficus had average 1527.2 µg/gm, 56.0 µg/gm and 56.09 µg/gm of Mn respectively.

Chromium is considerable as a serious pollutant due to wide industrial use (30). Chromium can cause nose irritation, respiratory damages and also liver and kidney and also it brings about alternation of genetical material (31) & Chromium level was very high in roadside soil 314.51 µg/gm against control value of 111.21 µg/gm. In grass it was 4.89 µg/gm and in ficus it was found to be 4.61 µg/gm against the control (Zero).

Nickel has been considerable to be as essential trace element for human and animal health (32). Due to bioaccumulation it shows skin irritation, damage to the lungs and nervous system (33). Ni level was considerable and was in roadside soil 85.2 µg/gm against control value 68.25 µg/gm. In grass it was 10.49 µg/gm and in ficus it was found to be 9.10 µg/gm against control 6.51 µg/gm.

Simple linear regression between the metals Viz, Pb, Cu, Ni, Mn, Zn, Cr and Cd present in the soil, grass and Ficus were calculated and are given in the tables 2&3. According to simple linear regression between the metal levels in roadside soil, grass and ficus were found in Zn, Cd, and Ni are

significant at 5% level (P>0.05). It may be indicating the bio concentration of these metals in the ficus, grass in addition to aerial deposition, This may attributed to the favourable root environment (34) i.e, Soil conditions might have favoured their absorption (35).

Correlations in case of chromium, nickel, manganese and copper contents between soil, grass and ficus were low due to low bioavailability of these metals owingto unfavourable root environment. Whatever excess content of these metals found in grass and ficus was presumed due to aerial deposition contributed by vehicular and other anthropogenic activities.

The elevated levels of heavy metals in roadside soil, ficus and grass are an indication of airborne pollutants of roadside environment of the urban area of Jamkhandi and surroundings. Soils have high retention capacity for the heavy metals are due to their cat ion exchange capacity (CEC), Complex organic substances, oxides and carbonates. Similar observations were also made by Tambavani and vathana (36) in *Azadirect indica* in madhurai city of southern region of Tamil Nadu.

The order increment of heavy metals in roadside is as follows:
In soil Mn > Cr > Zn > Pb > Ni > Cu > Cd
In grass Mn > Zn > Pb > Ni > Cr > Cu > Cd
In ficus Mn > Zn > Pb > Ni > Cu > Cr > Cd.

In soil the lesser mobility of metals and its accumulation on a long term basis , leads to overall higher concentration level of metals; where as in roadside ficus and grass, represents more recent accumulation due to new growth the substance followed by abscission of old parts and meteorological influences. Thus, the study of metal concentration of roadside soil, grass and ficus bordering the state highway, for livestock feeding may result in deleterious consequences from nutritional and veterinary hygienic point of view. The penetration of heavy metals into food chains due to vehicular emissions may cause a long range ecological and health hazards.

Acknowledgements

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi, India, and PG Department Botany, Karnatak University Dharwad (India) for providing necessary facilities to carry out research work.

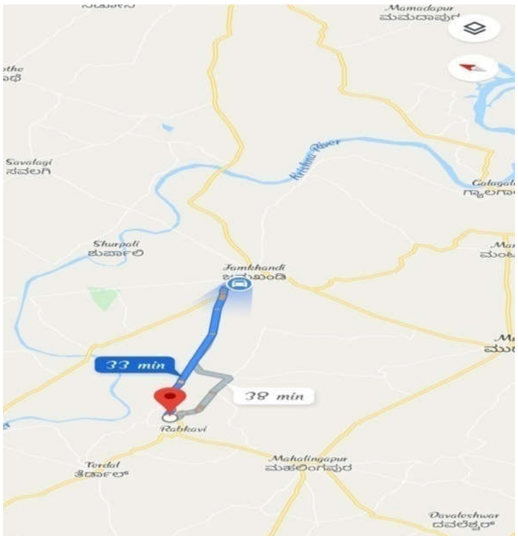

Fig 1 Map showing the state highway from Jamkhandi to Rabakavi-Banhatti.

Table 1 Sampling station along the state- highway from Jamkhandi to Rabakavi-Banhatti

Station No.	Sampling station	Nature of station
Control	Jamkhandi (City)	Unpolluted city vehicular movement is negligible
1	Hunnur	Unpolluted area with less distribution. Vehicular movement is high agricultural fields on either side of the road.
2	Madhurakhandi	Brick factories around and vehicular traffic is high
3	Bandigani cross	Vehicular movement is high with high vehicular traffic.
4	Yallatti	Vehicular movement is high with high vehicular Traffic.
5	Asangi (Near DEMP)	Brick factories around near to Rabkavi-Banhatti city with high vehicular traffic.
6	Rabakavi-Banhatti	Vehicular movement is high with high vehicular traffic.

Table 2 Metal accumulation profile in ficus, grass and soil

Sr. No.	Heavy metals	Control group ($\mu g\ g^{-1}$dry wt)	Roadside Ficus ($\mu g\ g^{-1}$ dry wt)		Roadside grass ($\mu g\ g^{-1}$ dry wt)		Control ($\mu g\ g^{-1}$dry wt)	Roadside soil ($\mu g\ g^{-1}$ dry wt)	
			Range	Mean ± SE	Range	Mean ± SE		Range	Mean ± SE
1	Lead	17.96	20.32-28.94	23.41±1.81	20.41-29.25	23.73±1.84	70.50	82.90-140.1	94.98±8.64
2	Copper	2.10	3.91-4.98	4.70±0.34	3.92-5.56	4.86±0.34	39.95	38.74-58.21	48.98±3.49
3	Zinc	15.91	24.21-35.7	32.54±3.81	24.20-34.5	32.87±3.10	29.89	32.29-389-51	187.9±53.25
4	Cadmium	0.81	1.11-1.74	1.39±0.07	1.20-1.82	1.57±0.081	2.13	1.75-2.89	2.0±0.18
5	Manganese	11.91	24.08-71.18	56.09±3.29	28.89-72.22	56.61±7.32	1251.4	1257.8-2058.5	1527.2±26.1
6	Chromium	ND	1.20-8.1	4.61±2.20	1.30-8.91	4.89±2.21	111.21	131.4-954.2	314.51±2.41
7	Nickel	6.51	8.1-148	9.10±1.40	8.7-15.1	10.49±1.41	68.25	70.49-108.4	85.2±5.74

*ND- Not detectable

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus. Significant at 5% P< 0.05)

Sl.No.	Metal	r-Value
1	Lead	0.638*
2	Copper	0.485
3	Zinc	0.824*
4	Cadmium	0.742*
5	Manganese	15.17
6	Nickel	6.61
7	Chromium	0.215

r = 0.60 and above have significant correlation

Table 4 Correlation of heavy metals in roadside soil and grass (Significant at 5% level (P< 0.05).

Sl. No.	Metal	r-Value
1	Lead	0.625*
2	Copper	0.499
3	Zinc	0.818*
4	Cadmium	0.699*
5	Manganese	0.524
6	Nickel	0.334
7	Chromium	0.214

r = 0.60 and above have significant correlation

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How to cite this article:

Rolli N.M *et al.*2019, Phytoassay of Heavy Metals Pollution in Roadside Environment: Bioindicators. *Int J Recent Sci Res.* 10(12), pp. 36499-36503. DOI: http://dx.doi.org/10.24327/ijrsr.2020.1012.4934

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ISSN: 0976-3031

Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(D), pp. 36499-36503, December, 2019

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4934

ARTICLE INFO

Article History:

Received 10th September, 2019
Received in revised form 2nd October, 2019
Accepted 26th November, 2019
Published online 28th December, 2019

Key Words:

Phytoassay, Bio indicators, Heavy metals, Food chain, anthropogenic activities, phytotool.

ABSTRACT

The Lead, Copper, Zinc Manganese, Nickel, Chromium and Cadmium contents in roadside grass, *Setaria verticellata* (L) P. Beaur (Family-Poaceae), *Ficus bengalensis* L. (Family- Moraceae) and soil from six sampling sites on state highway with heavy traffic loads passing through the city of Jamkhandi (Karnataka) were determined by atomic absorption spectrophotometer Results showed that soil, grass and *Ficus* contained elevated levels of the metals examined. Primarily it was found that the contamination occurs mainly by arial deposition of dust and the vehicular emissions. Apparently it was found that both soil and test plants can be utilized to reflect the roadside environment. The increased circulation of toxic metals in inevitable build-up of xenobiotic in food chain. The variation in heavy metal concentrations is due to changes in traffic density and anthropogenic activities. It is concluded that *Ficus* and *setaria* (grass) can be used as phytotool to monitor heavy metal pollution in roadside plants.

INTRODUCTION

Plants are important indicators of heavy metals environmental pollution (1). Environmental heavy metal pollution is mainly due to anthropogenic origin and results from the activities such as fossil fuels, vehicular emission, industrial emissions, landfill leachates, fertilizers, sewage and municipal wastes (2,3,4,5) Various plants have been used as bio indicators to assess the impact of a pollution source on the vicinity which is due to high metal accumulation of plants (6,7) worked on the basic criteria for the selection of species as a bio indicators. Now a days toxic effects of heavy metal are burning issue and been studied by many researchers (8,9). Entrance of heavy metals may occur in human and animal food chain as a results of their uptake by edible plants grown in an contaminated soil (10). The toxic and hazardous effects of some heavy metals on human health are very significant and may cause many fatal diseases. Lead (Pb) is one of the heavy metal that is responsible for anaemia, neurological disorder, hyperactivity and changes in blood enzymes in the human body (11) Cadmium and Zinc are important toxic metals & long time exposure of which causes renal pulmonary, hepatic, skeletal reproductive and many other carcinogenic effects (12,13) Many studies have been made on Pb, little attention has been focused on the contamination of other trace metals on the roadside environment. Metal such as iron, Copper, Zinc, Chromium (Vl), Cadmium, Manganese and Nickel are the essential components of many alloys, pipes, wires and tyres in motor vehicles and are released into the roadside environment as a result of mechanical abrasion Medicinal plants of Apocynaceae growing along the roadside have been employed as a phytotool to monitor toxic levels of heavy metals (14). The determination of heavy metal accumulation in roadside soil may be an index of the environmental pollution of Jamkhandi along the state highway towards Rabakavi & Banahatti. Keeping this view, the research was conducted to know the heavy metal accumulation of roadside soil, grass and *ficus* of the research area.

MATERIALS AND METHODS

Jamkhandi is the city of northern region of Karnataka (India) at longitude 16^0 30′ 6″ N and latitude 75^0 16′ 17″. It is well connected with Bagalkot and Vijayapur district of Karnataka state. The city and its surrounding places are suffered from high traffic density caused by vehicles. The grass (*Setaria*) and *Ficus* and soil were collected during summer 2018, which were three meters away from the state highway (Fig1 and table 1) passing from Jamkhandi to Rabhakavi Banhatti. Grass and ficus samples were collected from each site at three random spots that were spaced approximately at 1 m interval. The

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leaves were clipped with stainless steel scissors. All the samples of each site were then combined to give composite samples of about 300-500 g.

The leaves of grass (*Setaria)* and *Ficus* samples were dried at 80^0C for 48hr fine by powdered and sieved through 0.2mm sieve. One gram sample was digested using Gerhardt digestion unit using mixed acid digestion method. The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made upto 100ml.

Similarly, soil samples were dried, powdered and sieved through 0.2mm sieve. One gram of sample was digested Gerhardt digestion unit according to Allen *et al*. method (mixed acid digestion method). The resulting extracts were diluted and filtered through Whattman No 41 paper and made upto 100ml using double distilled water and analysed for heavy metal viz: Pb (Lead), Cd (Cadmium), Cu (Copper), Zn (Zinc), Mn (Manganese), Ni (Nickel) and Cr (Chromium) with GBC-932 plus Atomic Absorption Spectrometer (AAS) (Australia) with an air/ acetylene flame and metal hollow cathode lamps. Respective wavelengths were used for the estimation of solutions for heavy metals were purchased from Siscochemical Laboratory Bombay (1000 mg/L) for Cd 228.8 nm, Pb 217.0 nm, Ni 232.0 nm, Cu 324.7 nm, Zn 213.9 nm, Mn 279.5 nm and Cr 221.8 nm filters have been used for the estimation using AAS. The working standards were prepared by serial dilution of standard stock solutions and were for the calibration of the instrument.

RESULTS AND DISCUSSION

Environmental pollution with toxic metals has been dramatically increased since the increasing of vehicular exhausts (16). The pollution by heavy metals Viz, Pb, Cd, Cr, Ni, Mn, Zn etc, it is problem of concern (17). It is necessary to determine the kinds of environmental pollution and how for these exhibit and act as an efficient bio indicator in reducing the degree of pollution in the environment. The samples were collected along the state highway between Jamkhandi to Rabhakavi Banhatti for the estimation of heavy metals (Table.1).

The range arithmetic mean of heavy metal concentration of soil, ficus and grass samples of state highway and control sites are presented in Table 4. Correlation co-efficient of heavy metals in roadside soil, grass and ficus plant samples are given in the Table 3 and 4.

Lead is a poisonous metal in human it is directly absorbed into the blood stream and is stored in soft tissues, bones and teeth (18). The main source of Pb is exhaust fume**s** of automobiles, chimneys of factories, road side vehicles pollution (19). The results of our analysis shows that there are significant difference for lead between sampling sites in control the polluted area. Results shows that soil tends to accumulate more Pb than grass and the highest Pb level found in the roadside soil was 140.10µg /gm while for Ficus 28.94µg /gm and for the grass it was 29.25µg /gm. The mean soil Pb level is 94.98µg /gm indicated considerable contamination of the metal in the roadside environment, where as local soil control has baseline level of 70.50µg/gm Pb. The lead deposited on the vegetation reaches the soil by rain water from the surface and also by the death and decomposition of the plant. When incorporated in the soil Pb is of very low mobility. Hence, once contaminated a soil is liable to retain polluted with lead. The lead deposited in soil and vegetation can also cause enhanced levels of lead in soil (20,21).

Roadside soil gave higher Cu concentration due to industrial pollution near to the sampling location. The source of Cu being due to corrosion of metallic parts of car derived from engine wear brushing and bearing metals (22) Copper is essential element but higher concentration intake leads to severe mucosal irritation, wide spread capillary damage, renal and hepatic damage (23). The mean Cu level in road soil (48.98µg/gm) indicated considerable concentration of metal however, it was found to be much higher than the grass(4.70µg/gm) and ficus (4.86µg/gm).

The source of Zn in relation to automobile traffic is wearing of break lining, loses of oil and cooling liquid (24). Excess amount of Zn can cause in impairment of growth and reproduction. Excess Zn in the body bound in various transcription regions such as polymerase enzyme (25). Similar results were also reported by (26).

Cadmium is dispersed in natural environment through human activities as well as natural rock mineralization process, thus the plants can easily absorb Cd from the soil. The Cd in excess reported that the disruption in the transcription of genes in coding ribosomal proteins explains molecular mechanism of cadmium toxicity (27). Our analysis for Cd in the roadside plants and soil showed that there significant differences between polluted and control area. Cadmium level in roadside soil averaged about 2.0µgm. The mean Cd in ficus is 1.39 µg/gm and in grass 1.57 µg/gm. The results are in confirmation with the findings of Ho and Tai, (28).

Manganese is micronutrient essential for physiological functions but higher concentrations is toxic causing neuropsychiatic disorders (29). The soil grass and ficus contained much higher levels of Mn than other metals examined. The higher content may be attributed to the lithogenic factor apart from the vehicular pollution as indicated by the high values of Mn of control soil.The roadside soil, grass and ficus had average 1527.2 µg/gm, 56.0 µg/gm and 56.09 µg/gm of Mn respectively.

Chromium is considerable as a serious pollutant due to wide industrial use (30). Chromium can cause nose irritation, respiratory damages and also liver and kidney and also it brings about alternation of genetical material (31) & Chromium level was very high in roadside soil 314.51 µg/gm against control value of 111.21 µg/gm. In grass it was 4.89 µg/gm and in ficus it was found to be 4.61 µg/gm against the control (Zero).

Nickel has been considerable to be as essential trace element for human and animal health (32). Due to bioaccumulation it shows skin irritation, damage to the lungs and nervous system (33). Ni level was considerable and was in roadside soil 85.2 µg/gm against control value 68.25 µg/gm. In grass it was 10.49 µg/gm and in ficus it was found to be 9.10 µg/gm against control 6.51 µg/gm.

Simple linear regression between the metals Viz, Pb, Cu, Ni, Mn, Zn, Cr and Cd present in the soil, grass and Ficus were calculated and are given in the tables 2&3. According to simple linear regression between the metal levels in roadside soil, grass and ficus were found in Zn, Cd, and Ni are

significant at 5% level (P>0.05). It may be indicating the bio concentration of these metals in the ficus, grass in addition to aerial deposition, This may attributed to the favourable root environment (34) i.e, Soil conditions might have favoured their absorption (35).

Correlations in case of chromium, nickel, manganese and copper contents between soil, grass and ficus were low due to low bioavailability of these metals owingto unfavourable root environment. Whatever excess content of these metals found in grass and ficus was presumed due to aerial deposition contributed by vehicular and other anthropogenic activities.

The elevated levels of heavy metals in roadside soil, ficus and grass are an indication of airborne pollutants of roadside environment of the urban area of Jamkhandi and surroundings. Soils have high retention capacity for the heavy metals are due to their cat ion exchange capacity (CEC), Complex organic substances, oxides and carbonates. Similar observations were also made by Tambavani and vathana (36) in *Azadirect indica* in madhurai city of southern region of Tamil Nadu.

The order increment of heavy metals in roadside is as follows:
In soil Mn > Cr > Zn > Pb > Ni > Cu > Cd
In grass Mn > Zn > Pb > Ni > Cr > Cu > Cd
In ficus Mn > Zn > Pb > Ni > Cu > Cr > Cd.

In soil the lesser mobility of metals and its accumulation on a long term basis , leads to overall higher concentration level of metals; where as in roadside ficus and grass, represents more recent accumulation due to new growth the substance followed by abscission of old parts and meteorological influences. Thus, the study of metal concentration of roadside soil, grass and ficus bordering the state highway, for livestock feeding may result in deleterious consequences from nutritional and veterinary hygienic point of view. The penetration of heavy metals into food chains due to vehicular emissions may cause a long range ecological and health hazards.

Acknowledgements

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi, India, and PG Department Botany, Karnatak University Dharwad (India) for providing necessary facilities to carry out research work.

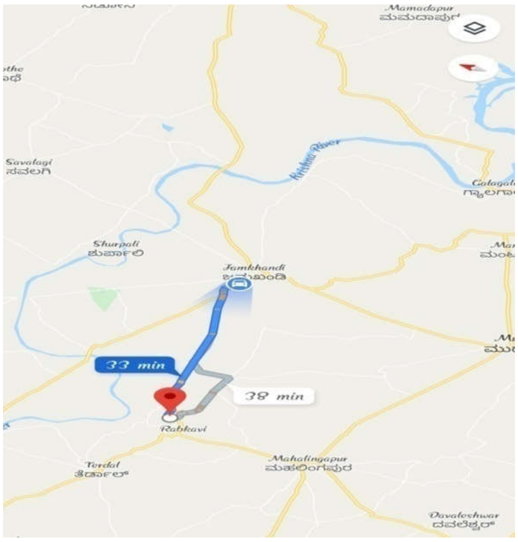

Fig 1 Map showing the state highway from Jamkhandi to Rabakavi-Banhatti.

Table 1 Sampling station along the state- highway from Jamkhandi to Rabakavi-Banhatti

Station No.	Sampling station	Nature of station
Control	Jamkhandi (City)	Unpolluted city vehicular movement is negligible
1	Hunnur	Unpolluted area with less distribution. Vehicular movement is high agricultural fields on either side of the road.
2	Madhurakhandi	Brick factories around and vehicular traffic is high
3	Bandigani cross	Vehicular movement is high with high vehicular traffic.
4	Yallatti	Vehicular movement is high with high vehicular Traffic.
5	Asangi (Near DEMP)	Brick factories around near to Rabkavi-Banhatti city with high vehicular traffic.
6	Rabakavi-Banhatti	Vehicular movement is high with high vehicular traffic.

Table 2 Metal accumulation profile in ficus, grass and soil

Sr. No.	Heavy metals	Control group ($\mu g\ g^{-1}$dry wt)	Roadside Ficus ($\mu g\ g^{-1}$ dry wt)		Roadside grass ($\mu g\ g^{-1}$ dry wt)		Control ($\mu g\ g^{-1}$dry wt)	Roadside soil ($\mu g\ g^{-1}$ dry wt)	
			Range	Mean ± SE	Range	Mean ± SE		Range	Mean ± SE
1	Lead	17.96	20.32-28.94	23.41±1.81	20.41-29.25	23.73±1.84	70.50	82.90-140.1	94.98±8.64
2	Copper	2.10	3.91-4.98	4.70±0.34	3.92-5.56	4.86±0.34	39.95	38.74-58.21	48.98±3.49
3	Zinc	15.91	24.21-35.7	32.54±3.81	24.20-34.5	32.87±3.10	29.89	32.29-389-51	187.9±53.25
4	Cadmium	0.81	1.11-1.74	1.39±0.07	1.20-1.82	1.57±0.081	2.13	1.75-2.89	2.0±0.18
5	Manganese	11.91	24.08-71.18	56.09±3.29	28.89-72.22	56.61±7.32	1251.4	1257.8-2058.5	1527.2±26.1
6	Chromium	ND	1.20-8.1	4.61±2.20	1.30-8.91	4.89±2.21	111.21	131.4-954.2	314.51±2.41
7	Nickel	6.51	8.1-148	9.10±1.40	8.7-15.1	10.49±1.41	68.25	70.49-108.4	85.2±5.74

*ND- Not detectable

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus. Significant at 5% P< 0.05)

Sl.No.	Metal	r-Value
1	Lead	0.638*
2	Copper	0.485
3	Zinc	0.824*
4	Cadmium	0.742*
5	Manganese	15.17
6	Nickel	6.61
7	Chromium	0.215

r = 0.60 and above have significant correlation

Table 4 Correlation of heavy metals in roadside soil and grass (Significant at 5% level (P< 0.05).

Sl. No.	Metal	r-Value
1	Lead	0.625*
2	Copper	0.499
3	Zinc	0.818*
4	Cadmium	0.699*
5	Manganese	0.524
6	Nickel	0.334
7	Chromium	0.214

r = 0.60 and above have significant correlation

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How to cite this article:

Rolli N.M *et al.*2019, Phytoassay of Heavy Metals Pollution in Roadside Environment: Bioindicators. *Int J Recent Sci Res.* 10(12), pp. 36499-36503. DOI: http://dx.doi.org/10.24327/ijrsr.2020.1012.4934

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ISSN: 0976-3031

Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(D), pp. 36499-36503, December, 2019

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOASSAY OF HEAVY METALS POLLUTION IN ROADSIDE ENVIRONMENT: BIOINDICATORS

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4934

ARTICLE INFO

Article History:

Received 10th September, 2019
Received in revised form 2nd October, 2019
Accepted 26th November, 2019
Published online 28th December, 2019

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Simple linear regression between the metals Viz, Pb, Cu, Ni, Mn, Zn, Cr and Cd present in the soil, grass and Ficus were calculated and are given in the tables 2&3. According to simple linear regression between the metal levels in roadside soil, grass and ficus were found in Zn, Cd, and Ni are

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The order increment of heavy metals in roadside is as follows:
In soil Mn > Cr > Zn > Pb > Ni > Cu > Cd
In grass Mn > Zn > Pb > Ni > Cr > Cu > Cd
In ficus Mn > Zn > Pb > Ni > Cu > Cr > Cd.

In soil the lesser mobility of metals and its accumulation on a long term basis , leads to overall higher concentration level of metals; where as in roadside ficus and grass, represents more recent accumulation due to new growth the substance followed by abscission of old parts and meteorological influences. Thus, the study of metal concentration of roadside soil, grass and ficus bordering the state highway, for livestock feeding may result in deleterious consequences from nutritional and veterinary hygienic point of view. The penetration of heavy metals into food chains due to vehicular emissions may cause a long range ecological and health hazards.

Acknowledgements

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi, India, and PG Department Botany, Karnatak University Dharwad (India) for providing necessary facilities to carry out research work.

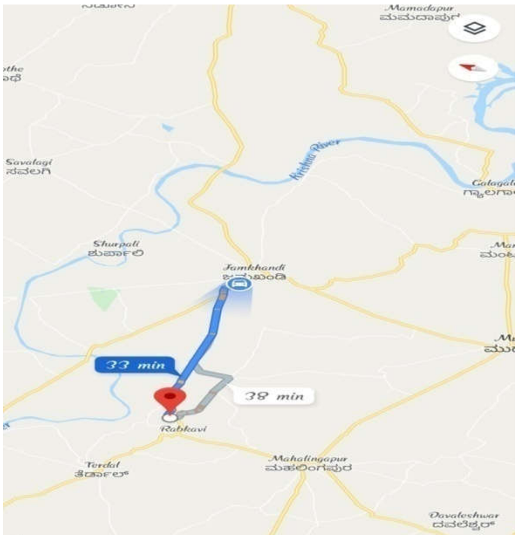

Fig 1 Map showing the state highway from Jamkhandi to Rabakavi-Banhatti.

Table 1 Sampling station along the state- highway from Jamkhandi to Rabakavi-Banhatti

Station No.	Sampling station	Nature of station
Control	Jamkhandi (City)	Unpolluted city vehicular movement is negligible
1	Hunnur	Unpolluted area with less distribution. Vehicular movement is high agricultural fields on either side of the road.
2	Madhurakhandi	Brick factories around and vehicular traffic is high
3	Bandigani cross	Vehicular movement is high with high vehicular traffic.
4	Yallatti	Vehicular movement is high with high vehicular Traffic.
5	Asangi (Near DEMP)	Brick factories around near to Rabkavi-Banhatti city with high vehicular traffic.
6	Rabakavi-Banhatti	Vehicular movement is high with high vehicular traffic.

Table 2 Metal accumulation profile in ficus, grass and soil

Sr. No.	Heavy metals	Control group (µg g^{-1}dry wt)	Roadside Ficus (µg g^{-1} dry wt)		Roadside grass (µg g^{-1} dry wt)		Control (µg g^{-1}dry wt)	Roadside soil (µg g^{-1} dry wt)	
			Range	Mean ± SE	Range	Mean ± SE		Range	Mean ± SE
1	Lead	17.96	20.32-28.94	23.41±1.81	20.41-29.25	23.73±1.84	70.50	82.90-140.1	94.98±8.64
2	Copper	2.10	3.91-4.98	4.70±0.34	3.92-5.56	4.86±0.34	39.95	38.74-58.21	48.98±3.49
3	Zinc	15.91	24.21-35.7	32.54±3.81	24.20-34.5	32.87±3.10	29.89	32.29-389-51	187.9±53.25
4	Cadmium	0.81	1.11-1.74	1.39±0.07	1.20-1.82	1.57±0.081	2.13	1.75-2.89	2.0±0.18
5	Manganese	11.91	24.08-71.18	56.09±3.29	28.89-72.22	56.61±7.32	1251.4	1257.8-2058.5	1527.2±26.1
6	Chromium	ND	1.20-8.1	4.61±2.20	1.30-8.91	4.89±2.21	111.21	131.4-954.2	314.51±2.41
7	Nickel	6.51	8.1-148	9.10±1.40	8.7-15.1	10.49±1.41	68.25	70.49-108.4	85.2±5.74

*ND- Not detectable

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus. Significant at 5% P< 0.05)

Sl.No.	Metal	r-Value
1	Lead	0.638*
2	Copper	0.485
3	Zinc	0.824*
4	Cadmium	0.742*
5	Manganese	15.17
6	Nickel	6.61
7	Chromium	0.215

r = 0.60 and above have significant correlation

Table 4 Correlation of heavy metals in roadside soil and grass (Significant at 5% level (P< 0.05).

Sl. No.	Metal	r-Value
1	Lead	0.625*
2	Copper	0.499
3	Zinc	0.818*
4	Cadmium	0.699*
5	Manganese	0.524
6	Nickel	0.334
7	Chromium	0.214

r = 0.60 and above have significant correlation

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How to cite this article:

Rolli N.M *et al*.2019, Phytoassay of Heavy Metals Pollution in Roadside Environment: Bioindicators. *Int J Recent Sci Res.* 10(12), pp. 36499-36503. DOI: http://dx.doi.org/10.24327/ijrsr.2020.1012.4934

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(D), pp. 36499-36503, December, 2019

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

PHYTOASSAY OF HEAVY METALS POLLUTION IN ROADSIDE ENVIRONMENT: BIOINDICATORS

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4934

ARTICLE INFO

Article History:

Received 10th September, 2019
Received in revised form 2nd October, 2019
Accepted 26th November, 2019
Published online 28th December, 2019

Key Words:

Phytoassay, Bio indicators, Heavy metals, Food chain, anthropogenic activities, phytotool.

ABSTRACT

The Lead, Copper, Zinc Manganese, Nickel, Chromium and Cadmium contents in roadside grass, *Setaria verticellata* (L) P. Beaur (Family-Poaceae), *Ficus bengalensis* L. (Family- Moraceae) and soil from six sampling sites on state highway with heavy traffic loads passing through the city of Jamkhandi (Karnataka) were determined by atomic absorption spectrophotometer Results showed that soil, grass and *Ficus* contained elevated levels of the metals examined. Primarily it was found that the contamination occurs mainly by arial deposition of dust and the vehicular emissions. Apparently it was found that both soil and test plants can be utilized to reflect the roadside environment. The increased circulation of toxic metals in inevitable build-up of xenobiotic in food chain. The variation in heavy metal concentrations is due to changes in traffic density and anthropogenic activities. It is concluded that *Ficus* and *setaria* (grass) can be used as phytotool to monitor heavy metal pollution in roadside plants.

INTRODUCTION

Plants are important indicators of heavy metals environmental pollution (1). Environmental heavy metal pollution is mainly due to anthropogenic origin and results from the activities such as fossil fuels, vehicular emission, industrial emissions, landfill leachates, fertilizers, sewage and municipal wastes (2,3,4,5) Various plants have been used as bio indicators to assess the impact of a pollution source on the vicinity which is due to high metal accumulation of plants (6,7) worked on the basic criteria for the selection of species as a bio indicators. Now a days toxic effects of heavy metal are burning issue and been studied by many researchers (8,9). Entrance of heavy metals may occur in human and animal food chain as a results of their uptake by edible plants grown in an contaminated soil (10). The toxic and hazardous effects of some heavy metals on human health are very significant and may cause many fatal diseases. Lead (Pb) is one of the heavy metal that is responsible for anaemia, neurological disorder, hyperactivity and changes in blood enzymes in the human body (11) Cadmium and Zinc are important toxic metals & long time exposure of which causes renal pulmonary, hepatic, skeletal reproductive and many other carcinogenic effects (12,13) Many studies have been made on Pb, little attention has been focused on the contamination of other trace metals on the roadside environment. Metal such as iron, Copper, Zinc, Chromium (VI), Cadmium, Manganese and Nickel are the essential components of many alloys, pipes, wires and tyres in motor vehicles and are released into the roadside environment as a result of mechanical abrasion Medicinal plants of Apocynaceae growing along the roadside have been employed as a phytotool to monitor toxic levels of heavy metals (14). The determination of heavy metal accumulation in roadside soil may be an index of the environmental pollution of Jamkhandi along the state highway towards Rabakavi & Banahatti. Keeping this view, the research was conducted to know the heavy metal accumulation of roadside soil, grass and *ficus* of the research area.

MATERIALS AND METHODS

Jamkhandi is the city of northern region of Karnataka (India) at longitude 16^0 30′ 6″ N and latitude 75^0 16′ 17″. It is well connected with Bagalkot and Vijayapur district of Karnataka state. The city and its surrounding places are suffered from high traffic density caused by vehicles. The grass (*Setaria*) and *Ficus* and soil were collected during summer 2018, which were three meters away from the state highway (Fig1 and table 1) passing from Jamkhandi to Rabhakavi Banhatti. Grass and ficus samples were collected from each site at three random spots that were spaced approximately at 1 m interval. The

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leaves were clipped with stainless steel scissors. All the samples of each site were then combined to give composite samples of about 300-500 g.

The leaves of grass (*Setaria)* and *Ficus* samples were dried at 80^0C for 48hr fine by powdered and sieved through 0.2mm sieve. One gram sample was digested using Gerhardt digestion unit using mixed acid digestion method. The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made upto 100ml.

Similarly, soil samples were dried, powdered and sieved through 0.2mm sieve. One gram of sample was digested Gerhardt digestion unit according to Allen *et al*. method (mixed acid digestion method). The resulting extracts were diluted and filtered through Whattman No 41 paper and made upto 100ml using double distilled water and analysed for heavy metal viz: Pb (Lead), Cd (Cadmium), Cu (Copper), Zn (Zinc), Mn (Manganese), Ni (Nickel) and Cr (Chromium) with GBC-932 plus Atomic Absorption Spectrometer (AAS) (Australia) with an air/ acetylene flame and metal hollow cathode lamps. Respective wavelengths were used for the estimation of solutions for heavy metals were purchased from Siscochemical Laboratory Bombay (1000 mg/L) for Cd 228.8 nm, Pb 217.0 nm, Ni 232.0 nm, Cu 324.7 nm, Zn 213.9 nm, Mn 279.5 nm and Cr 221.8 nm filters have been used for the estimation using AAS. The working standards were prepared by serial dilution of standard stock solutions and were for the calibration of the instrument.

RESULTS AND DISCUSSION

Environmental pollution with toxic metals has been dramatically increased since the increasing of vehicular exhausts (16). The pollution by heavy metals Viz, Pb, Cd, Cr, Ni, Mn, Zn etc, it is problem of concern (17). It is necessary to determine the kinds of environmental pollution and how for these exhibit and act as an efficient bio indicator in reducing the degree of pollution in the environment. The samples were collected along the state highway between Jamkhandi to Rabhakavi Banhatti for the estimation of heavy metals (Table.1).

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In grass Mn > Zn > Pb > Ni > Cr > Cu > Cd
In ficus Mn > Zn > Pb > Ni > Cu > Cr > Cd.

In soil the lesser mobility of metals and its accumulation on a long term basis , leads to overall higher concentration level of metals; where as in roadside ficus and grass, represents more recent accumulation due to new growth the substance followed by abscission of old parts and meteorological influences. Thus, the study of metal concentration of roadside soil, grass and ficus bordering the state highway, for livestock feeding may result in deleterious consequences from nutritional and veterinary hygienic point of view. The penetration of heavy metals into food chains due to vehicular emissions may cause a long range ecological and health hazards.

Acknowledgements

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi, India, and PG Department Botany, Karnatak University Dharwad (India) for providing necessary facilities to carry out research work.

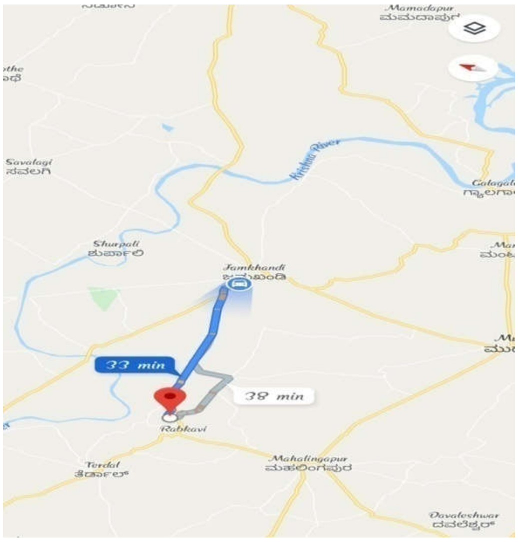

Fig 1 Map showing the state highway from Jamkhandi to Rabakavi-Banhatti.

Table 1 Sampling station along the state- highway from Jamkhandi to Rabakavi-Banhatti

Station No.	Sampling station	Nature of station
Control	Jamkhandi (City)	Unpolluted city vehicular movement is negligible
1	Hunnur	Unpolluted area with less distribution. Vehicular movement is high agricultural fields on either side of the road.
2	Madhurakhandi	Brick factories around and vehicular traffic is high
3	Bandigani cross	Vehicular movement is high with high vehicular traffic.
4	Yallatti	Vehicular movement is high with high vehicular Traffic.
5	Asangi (Near DEMP)	Brick factories around near to Rabkavi-Banhatti city with high vehicular traffic.
6	Rabakavi-Banhatti	Vehicular movement is high with high vehicular traffic.

Table 2 Metal accumulation profile in ficus, grass and soil

Sr. No.	Heavy metals	Control group (μg g⁻¹dry wt)	Roadside Ficus (μg g⁻¹ dry wt)		Roadside grass (μg g⁻¹ dry wt)		Control (μg g⁻¹dry wt)	Roadside soil (μg g⁻¹ dry wt)	
			Range	Mean ± SE	Range	Mean ± SE		Range	Mean ± SE
1	Lead	17.96	20.32-28.94	23.41±1.81	20.41-29.25	23.73±1.84	70.50	82.90-140.1	94.98±8.64
2	Copper	2.10	3.91-4.98	4.70±0.34	3.92-5.56	4.86±0.34	39.95	38.74-58.21	48.98±3.49
3	Zinc	15.91	24.21-35.7	32.54±3.81	24.20-34.5	32.87±3.10	29.89	32.29-389-51	187.9±53.25
4	Cadmium	0.81	1.11-1.74	1.39±0.07	1.20-1.82	1.57±0.081	2.13	1.75-2.89	2.0±0.18
5	Manganese	11.91	24.08-71.18	56.09±3.29	28.89-72.22	56.61±7.32	1251.4	1257.8-2058.5	1527.2±26.1
6	Chromium	ND	1.20-8.1	4.61±2.20	1.30-8.91	4.89±2.21	111.21	131.4-954.2	314.51±2.41
7	Nickel	6.51	8.1-148	9.10±1.40	8.7-15.1	10.49±1.41	68.25	70.49-108.4	85.2±5.74

*ND- Not detectable

Table 3 Correlation coefficient of heavy metals in roadside soil and ficus. Significant at 5% P< 0.05)

Sl.No.	Metal	r-Value
1	Lead	0.638*
2	Copper	0.485
3	Zinc	0.824*
4	Cadmium	0.742*
5	Manganese	15.17
6	Nickel	6.61
7	Chromium	0.215

r = 0.60 and above have significant correlation

Table 4 Correlation of heavy metals in roadside soil and grass (Significant at 5% level (P< 0.05).

Sl. No.	Metal	r-Value
1	Lead	0.625*
2	Copper	0.499
3	Zinc	0.818*
4	Cadmium	0.699*
5	Manganese	0.524
6	Nickel	0.334
7	Chromium	0.214

r = 0.60 and above have significant correlation

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How to cite this article:

Rolli N.M *et al.*2019, Phytoassay of Heavy Metals Pollution in Roadside Environment: Bioindicators. *Int J Recent Sci Res.* 10(12), pp. 36499-36503. DOI: http://dx.doi.org/10.24327/ijrsr.2020.1012.4934

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(A), pp. 36285-36291, December, 2019

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

TOXICITY EVALUATION OF LEAD IN AQUATIC MACROPHYTES

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4895

ARTICLE INFO

Article History:

Received 4th September, 2019
Received in revised form 25th October, 2019
Accepted 23rd November, 2019
Published online 28th December, 2019

Key Words:

Toxicity, Lead, Aquatic plants, Accumulation, Biochemical parameters, Symptoms.

ABSTRACT

The present study was focused on Lead (Pb) toxicity on macrophytes and biochemical parameters and profile of metal accumulation in aquatic macrophytes. The laboratory experiments were conducted for the assessment of Morphological Index Parameters (MIP), biochemical parameters and accumulation status of lead (Pb) in test plants at various concentrations, viz, 0.1, 0.5, 1.0, 1.5 and 2.0 ppm at regular interval for 12 days exposure duration. The test plants viz. *Salvinia,& Spirodela* were used for toxicity evaluation and profile of metal accumulation (Lead-Pb) from synthetic medium. The test plants were cultured in a modified Hoagland solution supplemented with $Pb(NO_3)_2$. The test plants shows visible symptoms like withering of roots, chlorosis, necrosis etc. particularly at higher concentrations i.e 1.5 ppm and 2.0 ppm, lower leaves gets decayed. However, at lower concentration i.e 0.1 ppm shows normal growth. The estimation of total chlorophyll, protein and carbohydrate of test plants showed significant increased at lower concentration i.e 0.1 ppm and decreased with increase in exposure concentrations i.e 0.5 to 2.0 ppm. It reveals that the toxic effect was directly proportional to its concentrations and exposure duration. The accumulation status was maximum in following orders (*Salvinia* > *Spirodela*) at low and higher concentrations of lead at 4 & 12 days exposure duration. However, accumulation profile in the test plants was maximum at 4 days exposure irrespective of metal concentrations and gradually decreases at subsequent exposure concentrations and duration.

INTRODUCTION

Heavy metal contamination in the water bodies is increasing at an alarming rate due to industrial and anthropogenic activities (1). Heavy metal pollution is a major environmental problem facing the modern word (1, 17). The danger of heavy metals is aggregated by their indefinite persistence in the environment because they cannot be destroyed biologically but are only transformed from oxidative state or organic complex to another. In addition, they are highly toxic for both aquatic flora and fauna (2). Heavy metals persisting in sediments may be slowly released into the water. Heavy metals viz, Zinc (Zn), Copper (Cu), Iron (Fe), Manganese (Mn)etc are represented as micronutrients (3) and are only toxic when taken in excess quantities, but nonessential ions like lead (Pb), Cadmium (Cd) and Nickel (Ni) inhibit various metabolic activities even in small quantities; (4, 5). The heavy metal lead (Pb) is selected as toxicant for the present study because it is used in several industries in India and are highly toxic to animals, humans and plants. Biological treatment of waste water through aquatic microphytes and macrophytes has great potential for its purification, which were effectively accumulates heavy metals (6). Aquatic macrophytes accumulate considerable amount of toxic metals and make the environment free from the xenobiotics. Thus, they play a significant role in cleaning up of environment and make it free from toxic pollutants. The metal tolerance of plants may be attributed to different enzymes, stress proteins and phytochelatins (7). Accumulation of metal at higher concentration causes retardation of biochemical activities and also generation of -SH group containing enzymes (8).

In the present investigation *Salvinia* and *Spirodela* common aquatic floating macrophytes, are used to study the effect of different concentrations of lead on morphology, biochemical constituents and efficiency in the accumulation of lead from the experimental pond under laboratory conditions.

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MATERIALS AND METHODS

Salvinia and *Spirodela* free floating aquatic plants from unpolluted water bodies is maintained in cement pots (1m diameter) under natural conditions at a temperature (28-30^{0}C). About 20g of young healthy *Salvinia,& Spirodela* were acclimatized for two weeks in Hoagland nutrient dolution maintaining pH between 7.1 to 7.4. The concentrations of lead in the polluted water are in the range of 0.1, 0.5, 1.0, 1.5 & 2.0 mg/l and tap water as a control. Morphological Index Parameter (MIP) viz, root length, leaf breadth and length were observed for 12 days at interval of 4 days. Photographs of test plants were taken by using Canon's Power Shot G_2 digital camera. For the further study the plants were harvested at the end of 4, 8 &12 days exposure and are thoroughly washed with distilled water and used for the estimation of total chlorophyll, protein and carbohydrates and also for morphological observations. Plants were harvested after 48 hours were dried at 80^{0}C for two days for metal extraction.

The fresh test plant samples of 1 g is macerated in 100 ml of 80% (v/v) chilled acetone by using pestle and mortar. The centrifuged and supernatant was used for the estimation of total chlorophyll by standard method (9) using 652 nm against the solvent (80% acetone as a blank). The protein was estimated by Lowry's method (10) using Bovine Serum Albumin (BSA) as a standard, using 660 nm and carbohydrates by phenol sulphuric acid method (11) using glucose as standard at 490 nm. Morphological characters were identified with the help of photographs, using Canon's Power Shot G_2 – digital camera.

The estimation of metal Pb in the test plant was carried out by using standard method (12). The dried and powdered 1 g plant material was digested by using mixed acid digestion method in Gerhardt digestion unit. The digested samples were diluted with double distilled water and filtered through Whatman filter paper No-14. The estimation of Pb was done by AAS (GBC 932 Plus Austrelia) with air acetylene oxidising flame and metal hollow cathode lamp at 217.00 nm wavelength. Working standards (SISCOP-Chem-Bombay Lab) were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values ± SE from two independent experiments with three replicates each. Data were subjected to Two – way ANOVA to know significance between concentrations and between exposure duration for the accumulation of heavy metal (Pb). Further, Dunet's test is also applied for multiple comparisons between control and other concentrations. Two – way ANOVA test is also extended to know the significance between concentrations and duration for biochemical parameters.

RESULTS AND DISCUSSION

Toxic effect of lead on Morphology

Morphometric assay is one of the quantitative tool for the assessment of toxicants on test plants was measured using Morphological Index Parameters (MIP). In test plants the rate of inhibition of growth in root and leaf is directly proportional to the concentration and exposure duration of lead.

The test plants showed luxuriant growth and was observed that slight increase in the laminal length and breadth at lower concentration (0.01 ppm) in test plants. In *Salvinia* at 0.1 ppm the lead was found to promote laminal length 1.633 ± 0.072, 1.766 ± 0.027, 1.933 ± 0.027, and breadth 1.833 ± 0.072, 1.900 ± 0.047, 2.00 ± 0.081 at 4, 8 and 12 days exposure. Similarly root length 4.33 ± 0.196, 4.566 ± 0.098, 4.666 ± 0.98 at 4, 8 and 12 days exposure in *Salvinia* at 0.1 ppm concentration. In *Spirodela* at 0.1 ppm Pb was found to promote laminal length 0.800 ± 0.047, 0.866 ± 0.027, 0.933 ± 0.027 and breadth 0.600 ±0.047, 0.633 ± 0.054, 0.933 ± 0.027 at 4,8 & 12 day exposure similarly root length 2.133 ± 0.072 and 2.300 ± 0.081 at 4 & 12 days exposure (Table. 1 & 2).

However, the higher concentration of Pb at 0.5 & 2.0 ppm exhibited toxicity symptoms like chlorosis, necrosis and fall of leaves was observed particularly at 2.0 ppm the roots gets wither away.

In *Salvinia* at 2.0 ppm Pb has severely inhibit the laminal length by 1.433 ± 0.047,1.300 ± 0.024, 0.966 ± 0.072 and breadth 1.400 ± 0.047, 1.166 ± 0.027, 0.933 ± 0.072 at 4, 8 & 12 days exposure. Similarly root length inhibition 3.366 ± 0.072, 2.300 ± 0.205 at 4 & 12 days exposure.

The test plants showed normal growth at their respective lower concentration i.e 0.1 ppm. Similar observations were made in *Limnentherum cristatum* at 1.0 ppm concentration of Pb, Zn and Cr (13) confirmed root elongation of test plants at lower concentrations of Cd in some members of *Lemnaceae.* However, the heavy metals induces morphological abnormalities in algae also (14). Similar observation is found in the laminal length of *Spirodela* at 2.0 ppm by 0.500 ± 0.00, 0.300 ± 0.00 at 4 &12 days of exposure duration and breadth to 0.466 ± 0.027 & 0.300 ± 0.00 at 4 & 12days of exposure duration. Root growth inhibition to 0.800 ± 0.047 & 0.666 ± 0.054 at 4 & 12 days of exposure duration (Table. 1 & 2).

Generally the rate of inhibition in root and leaf is directly proportional to the concentration of Pb in the test plants. Two way ANOVA test states that the concentrations are significantly toxic at 5% level but duration is not significant. MCA test also represents the maximum deviation at its higher concentration compared to control. The higher concentration of lead (0.5 – 2.0 ppm) exhibited toxicity symptoms like leaf fall, chlorosis etc. were observed. Our results of toxicity symptoms of Pb at high concentrations observed were similar to (15,16**)** and also in *Salvinia natanus* (17). The decrease in root is due to partial root damage due to some enzyme systems (18). Axtell (19) reported that absorption of lead by *Lemna minor* and the effect of Pb on tissues at higher concentrations.

Toxic effect of Pb on Biochemical Parameters

A number of heavy metals required by plants as a micronutrients and they act as a part of prosthetic groups and involved in a wide variety of metabolic activities. but higher concentration of heavy metals are toxic and induces physiological and genetical impairments in plants (20).

The total chlorophyll content was very sensitive to Pb toxicity. The results found that lead at 0.1 ppm found to augment chlorophyll synthesis and was directly proportional to concentration of synthetic medium and exposure duration in the test plants. In *Salvinia* the chlorophyll content was increased by 0.56% (0.712 mg/g), 0.66% (0.752mg/g) and 0.77% (0.782 mg/g) at 4 ,8 and 12 days exposure duration. In *Spirodela* the

chlorophyll content was increased by 1.39% (0.801 mg/g), 4.61 % (0.982 mg/g) and 6.39 % (1.164 mg/g) at 4,8 and 12 days of exposure duration respectively (Table 1 & 2).

Table 1 Effect of Lead on morphology of *Salvinia molesta*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control	3.833 ± 0.072	3.9 ± 0.355	3.966 ± 0.259	1.66 ± 0.0272	1.8 ± 0.094	1.7 ± 0.094	1.833 ± 0.072	1.733 ± 0.072	1.900 ± 0.047
0.1	4.333 ± 0.196	4.566 ± 0.098	4.666 ± 0.098	1.633 ± 0.072	1.833 ± 0.072	1.766 ± 0.027	1.900 ± 0.047	1.933 ± 0.027	2.000 ± 0.081
0.5	4.400 ± 0.309	4.300 ± 0.294	4.030 ± 0.294	1.633 ± 0.072	1.766 ± 0.072	1.633 ± 0.072	1.766 ± 0.047	1.633 ± 0.072	1.733 ± 0.027
1.0	3.966 ± 0.072	3.866 ± 0.072	3.566 ± 0.196	1.633 ± 0.072	1.733 ± 0.072	1.633 ± 0.072	1.633 ± 0.072	1.566 ± 0.027	1.333 ± 0.027
1.5	3.766 ± 0.118	3.700 ± 0.124	2.966 ± 0.241	1.500 ± 0.047	1.600 ± 0.094	1.500 ± 0.047	1.466 ± 0.027	1.366 ± 0.098	1.166 ± 0.072
2.0	3.366 ± 0.072	3.066 ± 0.027	2.3 ± 0.205	1.433 ± 0.047	1.4 ± 0.047	1.300 ± 0.124	1.166 ± 0.720	0.966 ± 0.072	0.933 ± 0.072

Values are expressed in cms
Mean values ± Standard Error

Table 2 Effect of Lead on morphology of *Spirodela polyrhiza*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
				Leaf size					
	Root length			Length	Breadth	Length	Breadth	Length	Breadth
Control 0	1.946 ± 0.124	1.9 ± 0.124	1.91 ± 0.124	0.633 ± 0.054	0.466 ± 0.027	0.633 ± 0.054	0.500 ± 0.047	0.630 ± 0.054	0.566 ± 0.027
0.1	2.133 ± 0.072	2.166 ± 0.098	2.300 ± 0.081	0.800 ± 0.047	0.600 ± 0.047	0.866 ± 0.027	0.633 ± 0.054	0.933 ± 0.027	0.666 ± 0.027
0.5	1.900 ± 0.081	1.766 ± 0.027	1.633 ± 0.098	0.633 ± 0.054	0.566 ± 0.027	0.633 ± 0.054	0.533 ± 0.027	0.633 ± 0.054	0.500 ± 0.047
1.0	1.500 ± 0.235	1.400 ± 0.188	1.266± 0.108	0.566 ± 0.027	0.500 ± 0.047	0.500 ± 0.047	0.500 ± 0.047	0.500 ± 0.047	0.466 ± 0.027
1.5	1.033 ± 0.072	0.900 ± 0.00	0.833 ± 0.027	0.533 ± 0.027	0.466 ± 0.027	0.466 ± 0.027	0.40 ± 0.00	0.433 ± 0.027	0.333 ± 0.027
2.0	0.800 ± 0.047	0.766 ± 0.027	0.666 ± 0.054	0.500 ± 0.00	0.466 ± 0.027	0.466 ± 0.027	0.366 ± 0.027	0.300 ± 0.00	0.300 ± 0.00

Values are expressed in cms
Mean values ± Standard Error

The stimulation of chlorophyll synthesis may be due to phytochelatins (PCs) which play important role in detoxification of Pb (21). Phytochelatins also important role in cellular metal ion in homeostasis and detoxification (22).

However, the higher concentration of Pb found to inhibit the chlorophyll synthesis in the test plant. The inhibition at 2.0 ppm of Pb 19.13 % (0.569 mg/g) 25.70 % (0.555mg/g) and 34.79 % (0.506 mg/g) significant at $p > 0.95\%$ in *Salvinia*, inhibition at 2.0 ppm Pb by 5.44 % (0.747 mg/g) 40.76 % (0.539mg/g) and 72.44% (0.534 mg/g) in *Spirodela* respectively at 4,8 & 12 days of exposure compared to control. Two way ANOVA represents biochemical toxicity to the test plants, the concentrations were significant at $p > 0.01$ level but duration is not significant (Table 3 & 4).

Table 3 Two way ANOVA for biochemical effects of Lead on *Salvinia molesta*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	20.420**	7.153**	46.149**
F- value (between duration)	0.449	0.805	1.732

** Significant at P < 0.01 level

Table 4 Two way ANOVA for biochemical effects of Lead on *Spriodela polyrhiza*

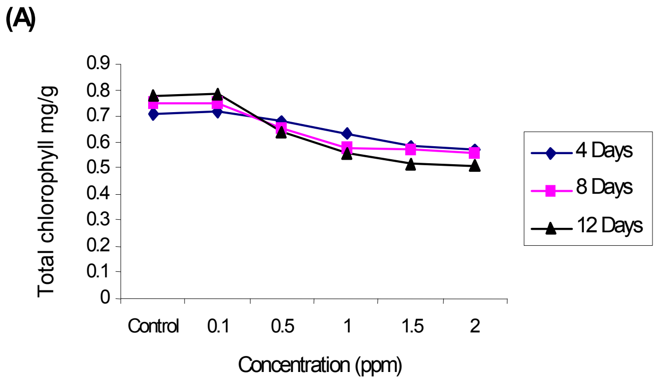
	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	4.352**	6.966**	11.91**
F- value (between duration)	0.239	0.982	6.67

** Significant at P < 0.01 level

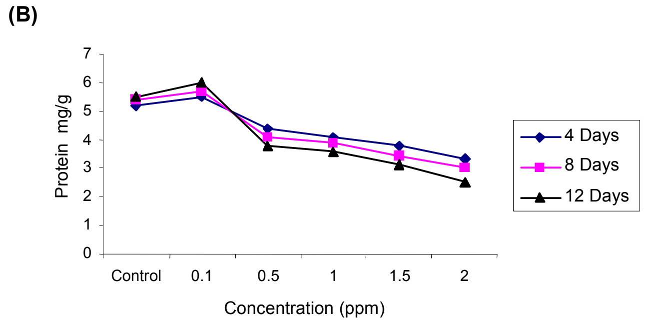
However, higher concentration (0.5, 1.0, 1.5 & 2.0 ppm) of Pb was found to inhibit chlorophyll synthesis. The inhibition of chlorophyll at higher concentration (2.0 ppm) of Pb by 34.79 % in *Salvinia*,& 72.44 % in *Spirodela* at 12 days exposure compared to their respective control.

The decline in chlorophyll content in plants exposed to Pb due to i) inhibition of important enzymes associated with chlorophyll biosynthesis ii) peroxidation of chloroplast membranes from heavy metal induced oxidative stress and iii) formation of metal stimulated chlorophyll (23). This inhibition activity of Pb is due to inhibition of haemobiosynthesis and formation of chlorophyll by integrating with functional –SH group of enzyme involved in the biosynthesis of chlorophyll (24). Similar observation was made by Singh (25) in *Hydrilla verticillata* at higher concentration of Pb at 2.0 ppm and 0.5 ppm of Cadmium. The presence of Pb decreases chlorophyll and caretonoids in *Brassica rapanus* (26). Similarly the synthesis and level of chlorophyll decreased in other plant species under the influence of Pb and Cd (27). The total chlorophyll content of experimental plants at higher concentration significantly decreased with respect to exposure duration.

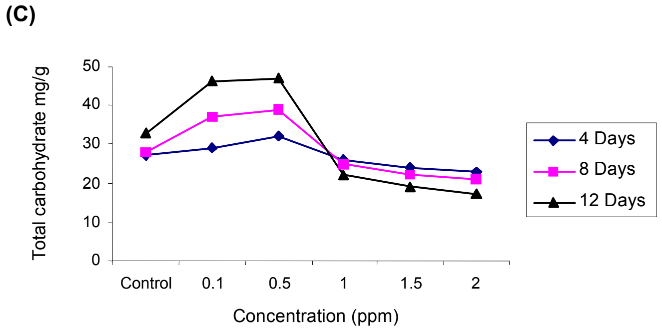
Carbohydrates acts as osmoregulators which maintains water balance in plants (28). Lower concentration (0.1 ppm) of Pb increases carbohydrate content from 7.40 % (29.0 mg/g) 32.14 % (37.0mg/g) and 39.39 % (46.0 mg/g) in *Salvinia*, and 3.22% (32.0mg/g) 26.47 % (43mg/g) and 33.33% (53.0mg/g) in *Spirodela* at 4,8 and 12 days exposure duration compared to control. Thus the percent enhancement of carbohydrate at 12 days exposure is 39.39 % in *Salvinia*, & 39.33 % in *Spirodela* However, the higher concentration of Pb inhibits the synthesis of carbohydrate and was vary from 23 mg/g to 17 mg/g in *Salvinia* 26 mg/g to 18 mg/g in *Spirodela* at 4 and 12 days exposure. The reduction in carbohydrate content can be attributed to the reduced rates of photochemical activities (14) and also Succinate Dehydrogenase (SDH) fall in cells indicate oxygen stress and energy crisis and mitochondrial disturbances (29). Generally heavy metals damages the photosynthesis apparatus in particular the harvesting complex II (23) and photosynthesis I & II (27) (Fig. 1 & 2). The protein synthesis at 0.1 ppm of Pb was promotive irrespective exposure duration in the test plants. However, the protein content was decreased at subsequent concentrations and inhibition was also directly proportional to the exposure duration also.



(A) Total Chlorophyll



(B) Carbohydrate

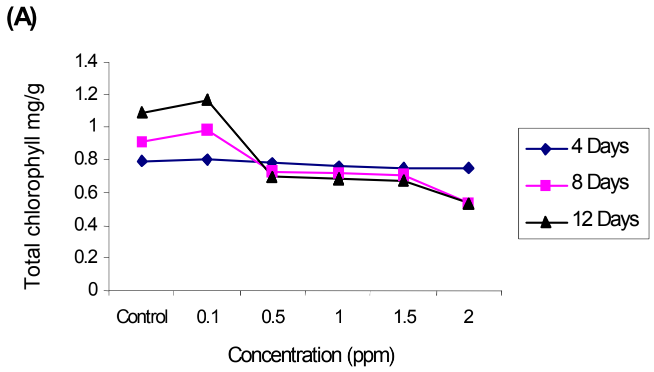


(C) Protein

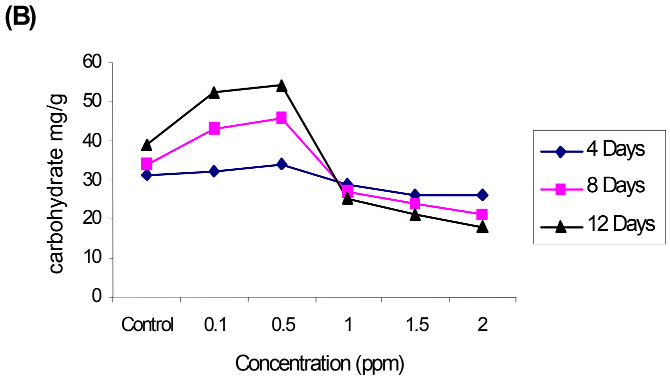
Fig 1 Biochemical effects of Lead on *Salvinia molesta*

The 0.1 ppm of Pb promoted the protein synthesis by 5.76 % (5.5 mg/g), 5.46 % (5.7mg/g) and 9.09% (6.0 mg/g) in *Salvinia*, 6.30% (8.4 mg/g), 11.11 % (9.0mg/g) and 15.2 % (14.4 mg/g) *Spirodela* at 4,8 and 12 days exposure duration respectively compared to control. The stimulation of protein synthesis at lower concentration of Pb may be altered to the synthesis of stress proteins (30). The phytochelatins (PCs) are produced by Glutathione Reductase (GR) and Phytochelatin Synthetase (PS). These proteins bind and regulate the Pb and sequesters the Pb toxicity and the plants shows the metal tolerance (31).

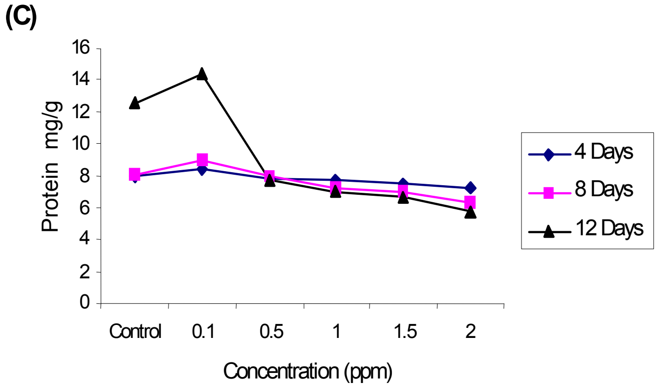
However, our investigation revealed that higher concentration of 'Pb' inhibit protein metabolism in experimental plants. The inhibition of protein content increase 36.53 % (3.3 mg/g), 44.44 % (3.0mg/g) and 54.54 % (2.5 mg/g) in *Salvinia* and 8.86 % (7.2 mg/g), 22.22% (6.3mg/g) and 53.6 % (5.8 mg/g) in *Spirodela* was noticed at 4,8 and 12 days exposure. The Cd shows slight inhibitory effect at 0.5 ppm and severe inhibition of algal growth at higher concentration in some algae (32). The DNA and RNA were inhibited, rather due to blocking of –SH group or to the inactivity of RNA and DNA polymerase activity (32) (Fig. 1 & 2).



(A) Total Chlorophyll



(B) Carbohydrate



(C) Protein

Fig 2 Biochemical effects of Lead on *Spirodela polyrhiza*

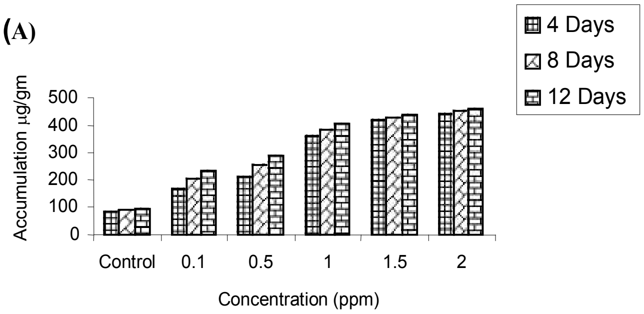
Application of two-way ANOVA is found that the biochemical responses of test plants species with respect to their concentrations were significant at $p > 0.01$ level. however, the exposure durations are not statistically significant (Table 3 & 4).

Profile of Metal Accumulation

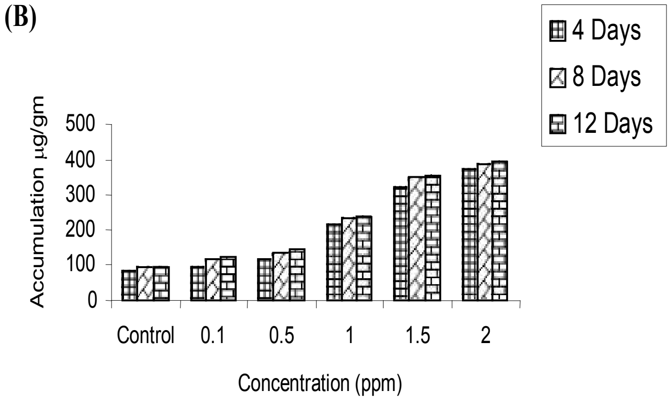
Heavy metal pollution of water is a major environmental concern, is increasing at alarming rate due to anthropogenic activities and is drawing attention and gaining paramanual importance due to its obvious impact on health through the food chain (1,33).

Fig. (3) shows the concentration of Pb accumulation in *Salvinia*,& *Spirodela*. The *Salvinia* grown in experimental pond containing 0.1 ppm found to accumulate 168 µg/g, 205 µg/g, and 231 µg/g and in *Spirodela* it is about 96 µg/g, 114 µg/g and 123 µg/g at 4,8 and 12 days exposure duration respectively. Generally in our experiments it was found that the rate of accumulation is maximum at 4 days exposure irrespective of concentrations and exposure duration, however, at subsequent concentrations and exposure durations it is marginal. Similar observations were also made by Aslam (34), in *Nastutium officinate* and *Mentha aquatica* to the exposure concentrations of 0.1 and 0.5 ppm of Cd. Similar observation was made by Sinha & Pandey (35) in the accumulation of Ni in *Hydrilla verticillata* and Cd and Pb in *Salvinia cuculata*. The increase in the accumulation might be due to increased number of binding sites for the completion of number of heavy metal ions leading to the increased absorption. Brenda (36) was also observed dramatic uptake of Zn in *Cladophora glomerata* within first minutes.

However, the higher concentration (2.0 ppm) of Pb accumulation in *Salvinia* by 443 µg/g,458 /g and 460 µg/g and in *Spirodela* by 374 µg/g , 391 µg/g and 395 µg/g during 4,8 and 12 days exposure duration respectively. The increase in the accumulation might be due to increased number of binding sites for the complexation of heavy metal ions, leading to the increased observation, however, slow accumulation may be due to binding ions to the plants and establishment of equilibrium status between adsorbate and adsorbant (33,37,38).



(A) ***Salvinia***



(B) ***Spirodela***

Fig 3 Accumulation profile of Lead by aquatic macrophytes

Generally (39, 40) reported that the accumulation of metal by aquatic macrophytes under controlled laboratory condition was dependent on metal concentration in the water. Generally it was found that plants exposed to concentration of 0.1 ppm of Pb found to accumulate maximum in *Salvinia* (23 µg/g), *Sporodela* (123 µg/g) during 12 days exposure duration followed by *Salvinia*. Similarly at high concentration of 2.0 ppm Pb *Salvinia* accumulates maximum of Pb (460 µg/g) followed by *Spirodela* (395 µg/g) during 12 days exposure duration (Fig. 3).

The initial increase in the accumulation by macrophytes may be due to increased number of binding sites for the complexation of heavy metal ions leading to the increased absorption. However, slow removal beyond an optimum dose may be attributed to the binding of almost all ions to the plants and the establishment of equilibrium between adsorbate and adsoibant at the existing operating conditions (38).

The *Spirodela* is found to be a suitable candidate for toxicity evaluation. The *Salvinia* is the most tolerant species and can be used for the remediation of heavy metals from the aquastic ecosystem and environmental monitoring.

Two-way ANOVA showed that both concentration and exposure duration were significant at p < 0.01 level in test plants and further Dunet's test was also applied for multiple comparison between control and different concentration treatments of test plants. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table. 5).

Table 5 Two way ANOVA with Dunet's test for multiple comparison for accumulation of Lead by aquatic macrophytes

	Salvinia	Spirodela
F-Value (between concentration)	376.56**	2558.17**
F- value (between duration)	13.54**	45.74**
Dunet's Value	20.54	6.87
Control V/s 0.1ppm	112.66	21.33
Control V/s 0.5ppm	162.33	40.33
Control V/s 1.0ppm	294.00	141.00
Control V/s 1.5ppm	342.00	251.00
Control V/s 2.0ppm	365.00	297.00

** Significant at P < 0.01 level

Acknowledgement

The authors are thankful to the Principal BLDEA's Degree College Jamkhandi. INDIA, Research and Development Centre, Bharthiar University Coimbatore and JSS College Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in the references of this manuscript. The authors are also grateful to editors, publishers of all those articles, journals and books from where the literature of this article has been received and discussed

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How to cite this article:

Rolli.N.M et al.2019, Toxicity Evaluation of Lead In Aquatic Macrophytes. *Int J Recent Sci Res.* 10(12), pp. 36285-36291. DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4895

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Available Online at http://www.recentscientific.com

CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(A), pp. 36285-36291, December, 2019

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

TOXICITY EVALUATION OF LEAD IN AQUATIC MACROPHYTES

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4895

ARTICLE INFO

Article History:

Received 4th September, 2019
Received in revised form 25th October, 2019
Accepted 23rd November, 2019
Published online 28th December, 2019

Key Words:

Toxicity, Lead, Aquatic plants, Accumulation, Biochemical parameters, Symptoms.

ABSTRACT

The present study was focused on Lead (Pb) toxicity on macrophytes and biochemical parameters and profile of metal accumulation in aquatic macrophytes. The laboratory experiments were conducted for the assessment of Morphological Index Parameters (MIP), biochemical parameters and accumulation status of lead (Pb) in test plants at various concentrations, viz, 0.1, 0.5, 1.0, 1.5 and 2.0 ppm at regular interval for 12 days exposure duration. The test plants viz. *Salvinia,& Spirodela* were used for toxicity evaluation and profile of metal accumulation (Lead-Pb) from synthetic medium. The test plants were cultured in a modified Hoagland solution supplemented with $Pb(NO_3)_2$. The test plants shows visible symptoms like withering of roots, chlorosis, necrosis etc. particularly at higher concentrations i.e 1.5 ppm and 2.0 ppm, lower leaves gets decayed. However, at lower concentration i.e 0.1 ppm shows normal growth. The estimation of total chlorophyll, protein and carbohydrate of test plants showed significant increased at lower concentration i.e 0.1 ppm and decreased with increase in exposure concentrations i.e 0.5 to 2.0 ppm. It reveals that the toxic effect was directly proportional to its concentrations and exposure duration. The accumulation status was maximum in following orders (*Salvinia* > *Spirodela*) at low and higher concentrations of lead at 4 & 12 days exposure duration. However, accumulation profile in the test plants was maximum at 4 days exposure irrespective of metal concentrations and gradually decreases at subsequent exposure concentrations and duration.

INTRODUCTION

Heavy metal contamination in the water bodies is increasing at an alarming rate due to industrial and anthropogenic activities (1). Heavy metal pollution is a major environmental problem facing the modern word (1, 17). The danger of heavy metals is aggregated by their indefinite persistence in the environment because they cannot be destroyed biologically but are only transformed from oxidative state or organic complex to another. In addition, they are highly toxic for both aquatic flora and fauna (2). Heavy metals persisting in sediments may be slowly released into the water. Heavy metals viz, Zinc (Zn), Copper (Cu), Iron (Fe), Manganese (Mn)etc are represented as micronutrients (3) and are only toxic when taken in excess quantities, but nonessential ions like lead (Pb), Cadmium (Cd) and Nickel (Ni) inhibit various metabolic activities even in small quantities; (4, 5). The heavy metal lead (Pb) is selected as toxicant for the present study because it is used in several industries in India and are highly toxic to animals, humans and plants. Biological treatment of waste water through aquatic microphytes and macrophytes has great potential for its purification, which were effectively accumulates heavy metals (6). Aquatic macrophytes accumulate considerable amount of toxic metals and make the environment free from the xenobiotics. Thus, they play a significant role in cleaning up of environment and make it free from toxic pollutants. The metal tolerance of plants may be attributed to different enzymes, stress proteins and phytochelatins (7). Accumulation of metal at higher concentration causes retardation of biochemical activities and also generation of -SH group containing enzymes (8).

In the present investigation *Salvinia* and *Spirodela* common aquatic floating macrophytes, are used to study the effect of different concentrations of lead on morphology, biochemical constituents and efficiency in the accumulation of lead from the experimental pond under laboratory conditions.

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MATERIALS AND METHODS

Salvinia and *Spirodela* free floating aquatic plants from unpolluted water bodies is maintained in cement pots (1m diameter) under natural conditions at a temperature (28-30^{0}C). About 20g of young healthy *Salvinia,& Spirodela* were acclimatized for two weeks in Hoagland nutrient dolution maintaining pH between 7.1 to 7.4. The concentrations of lead in the polluted water are in the range of 0.1, 0.5, 1.0, 1.5 & 2.0 mg/l and tap water as a control. Morphological Index Parameter (MIP) viz, root length, leaf breadth and length were observed for 12 days at interval of 4 days. Photographs of test plants were taken by using Canon's Power Shot G_2 digital camera. For the further study the plants were harvested at the end of 4, 8 &12 days exposure and are thoroughly washed with distilled water and used for the estimation of total chlorophyll, protein and carbohydrates and also for morphological observations. Plants were harvested after 48 hours were dried at 80^{0}C for two days for metal extraction.

The fresh test plant samples of 1 g is macerated in 100 ml of 80% (v/v) chilled acetone by using pestle and mortar. The centrifuged and supernatant was used for the estimation of total chlorophyll by standard method (9) using 652 nm against the solvent (80% acetone as a blank). The protein was estimated by Lowry's method (10) using Bovine Serum Albumin (BSA) as a standard, using 660 nm and carbohydrates by phenol sulphuric acid method (11) using glucose as standard at 490 nm. Morphological characters were identified with the help of photographs, using Canon's Power Shot G_2 – digital camera.

The estimation of metal Pb in the test plant was carried out by using standard method (12). The dried and powdered 1 g plant material was digested by using mixed acid digestion method in Gerhardt digestion unit. The digested samples were diluted with double distilled water and filtered through Whatman filter paper No-14. The estimation of Pb was done by AAS (GBC 932 Plus Austrelia) with air acetylene oxidising flame and metal hollow cathode lamp at 217.00 nm wavelength. Working standards (SISCOP-Chem-Bombay Lab) were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values ± SE from two independent experiments with three replicates each. Data were subjected to Two – way ANOVA to know significance between concentrations and between exposure duration for the accumulation of heavy metal (Pb). Further, Dunet's test is also applied for multiple comparisons between control and other concentrations. Two – way ANOVA test is also extended to know the significance between concentrations and duration for biochemical parameters.

RESULTS AND DISCUSSION

Toxic effect of lead on Morphology

Morphometric assay is one of the quantitative tool for the assessment of toxicants on test plants was measured using Morphological Index Parameters (MIP). In test plants the rate of inhibition of growth in root and leaf is directly proportional to the concentration and exposure duration of lead.

The test plants showed luxuriant growth and was observed that slight increase in the laminal length and breadth at lower concentration (0.01 ppm) in test plants. In *Salvinia* at 0.1 ppm the lead was found to promote laminal length 1.633 ± 0.072, 1.766 ± 0.027, 1.933 ± 0.027, and breadth 1.833 ± 0.072, 1.900 ± 0.047, 2.00 ± 0.081 at 4, 8 and 12 days exposure. Similarly root length 4.33 ± 0.196, 4.566 ± 0.098, 4.666 ± 0.98 at 4, 8 and 12 days exposure in *Salvinia* at 0.1 ppm concentration. In *Spirodela* at 0.1 ppm Pb was found to promote laminal length 0.800 ± 0.047, 0.866 ± 0.027, 0.933 ± 0.027 and breadth 0.600 ±0.047, 0.633 ± 0.054, 0.933 ± 0.027 at 4,8 & 12 day exposure similarly root length 2.133 ± 0.072 and 2.300 ± 0.081 at 4 & 12 days exposure (Table. 1 & 2).

However, the higher concentration of Pb at 0.5 & 2.0 ppm exhibited toxicity symptoms like chlorosis, necrosis and fall of leaves was observed particularly at 2.0 ppm the roots gets wither away.

In *Salvinia* at 2.0 ppm Pb has severely inhibit the laminal length by 1.433 ± 0.047,1.300 ± 0.024, 0.966 ± 0.072 and breadth 1.400 ± 0.047, 1.166 ± 0.027, 0.933 ± 0.072 at 4, 8 & 12 days exposure. Similarly root length inhibition 3.366 ± 0.072, 2.300 ± 0.205 at 4 & 12 days exposure.

The test plants showed normal growth at their respective lower concentration i.e 0.1 ppm. Similar observations were made in *Limnentherum cristatum* at 1.0 ppm concentration of Pb, Zn and Cr (13) confirmed root elongation of test plants at lower concentrations of Cd in some members of *Lemnaceae.* However, the heavy metals induces morphological abnormalities in algae also (14). Similar observation is found in the laminal length of *Spirodela* at 2.0 ppm by 0.500 ± 0.00, 0.300 ± 0.00 at 4 &12 days of exposure duration and breadth to 0.466 ± 0.027 & 0.300 ± 0.00 at 4 & 12days of exposure duration. Root growth inhibition to 0.800 ± 0.047 & 0.666 ± 0.054 at 4 & 12 days of exposure duration (Table. 1 & 2).

Generally the rate of inhibition in root and leaf is directly proportional to the concentration of Pb in the test plants. Two way ANOVA test states that the concentrations are significantly toxic at 5% level but duration is not significant. MCA test also represents the maximum deviation at its higher concentration compared to control. The higher concentration of lead (0.5 – 2.0 ppm) exhibited toxicity symptoms like leaf fall, chlorosis etc. were observed. Our results of toxicity symptoms of Pb at high concentrations observed were similar to (15,16**)** and also in *Salvinia natanus* (17). The decrease in root is due to partial root damage due to some enzyme systems (18). Axtell (19) reported that absorption of lead by *Lemna minor* and the effect of Pb on tissues at higher concentrations.

Toxic effect of Pb on Biochemical Parameters

A number of heavy metals required by plants as a micronutrients and they act as a part of prosthetic groups and involved in a wide variety of metabolic activities. but higher concentration of heavy metals are toxic and induces physiological and genetical impairments in plants (20).

The total chlorophyll content was very sensitive to Pb toxicity. The results found that lead at 0.1 ppm found to augment chlorophyll synthesis and was directly proportional to concentration of synthetic medium and exposure duration in the test plants. In *Salvinia* the chlorophyll content was increased by 0.56% (0.712 mg/g), 0.66% (0.752mg/g) and 0.77% (0.782 mg/g) at 4 ,8 and 12 days exposure duration. In *Spirodela* the

chlorophyll content was increased by 1.39% (0.801 mg/g), 4.61 % (0.982 mg/g) and 6.39 % (1.164 mg/g) at 4,8 and 12 days of exposure duration respectively (Table 1 & 2).

Table 1 Effect of Lead on morphology of *Salvinia molesta*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control	3.833 ± 0.072	3.9 ± 0.355	3.966 ± 0.259	1.66 ± 0.0272	1.8 ± 0.094	1.7 ± 0.094	1.833 ± 0.072	1.733 ± 0.072	1.900 ± 0.047
0.1	4.333 ± 0.196	4.566 ± 0.098	4.666 ± 0.098	1.633 ± 0.072	1.833 ± 0.072	1.766 ± 0.027	1.900 ± 0.047	1.933 ± 0.027	2.000 ± 0.081
0.5	4.400 ± 0.309	4.300 ± 0.294	4.030 ± 0.294	1.633 ± 0.072	1.766 ± 0.072	1.633 ± 0.072	1.766 ± 0.047	1.633 ± 0.072	1.733 ± 0.027
1.0	3.966 ± 0.072	3.866 ± 0.072	3.566 ± 0.196	1.633 ± 0.072	1.733 ± 0.072	1.633 ± 0.072	1.633 ± 0.072	1.566 ± 0.027	1.333 ± 0.027
1.5	3.766 ± 0.118	3.700 ± 0.124	2.966 ± 0.241	1.500 ± 0.047	1.600 ± 0.094	1.500 ± 0.047	1.466 ± 0.027	1.366 ± 0.098	1.166 ± 0.072
2.0	3.366 ± 0.072	3.066 ± 0.027	2.3 ± 0.205	1.433 ± 0.047	1.4 ± 0.047	1.300 ± 0.124	1.166 ± 0.720	0.966 ± 0.072	0.933 ± 0.072

Values are expressed in cms
Mean values ± Standard Error

Table 2 Effect of Lead on morphology of *Spirodela polyrhiza*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
				Leaf size					
	Root length			Length	Breadth	Length	Breadth	Length	Breadth
Control 0	1.946 ± 0.124	1.9 ± 0.124	1.91 ± 0.124	0.633 ± 0.054	0.466 ± 0.027	0.633 ± 0.054	0.500 ± 0.047	0.630 ± 0.054	0.566 ± 0.027
0.1	2.133 ± 0.072	2.166 ± 0.098	2.300 ± 0.081	0.800 ± 0.047	0.600 ± 0.047	0.866 ± 0.027	0.633 ± 0.054	0.933 ± 0.027	0.666 ± 0.027
0.5	1.900 ± 0.081	1.766 ± 0.027	1.633 ± 0.098	0.633 ± 0.054	0.566 ± 0.027	0.633 ± 0.054	0.533 ± 0.027	0.633 ± 0.054	0.500 ± 0.047
1.0	1.500 ± 0.235	1.400 ± 0.188	1.266± 0.108	0.566 ± 0.027	0.500 ± 0.047	0.500 ± 0.047	0.500 ± 0.047	0.500 ± 0.047	0.466 ± 0.027
1.5	1.033 ± 0.072	0.900 ± 0.00	0.833 ± 0.027	0.533 ± 0.027	0.466 ± 0.027	0.466 ± 0.027	0.40 ± 0.00	0.433 ± 0.027	0.333 ± 0.027
2.0	0.800 ± 0.047	0.766 ± 0.027	0.666 ± 0.054	0.500 ± 0.00	0.466 ± 0.027	0.466 ± 0.027	0.366 ± 0.027	0.300 ± 0.00	0.300 ± 0.00

Values are expressed in cms
Mean values ± Standard Error

The stimulation of chlorophyll synthesis may be due to phytochelatins (PCs) which play important role in detoxification of Pb (21). Phytochelatins also important role in cellular metal ion in homeostasis and detoxification (22).

However, the higher concentration of Pb found to inhibit the chlorophyll synthesis in the test plant. The inhibition at 2.0 ppm of Pb 19.13 % (0.569 mg/g) 25.70 % (0.555mg/g) and 34.79 % (0.506 mg/g) significant at p > 0.95% in *Salvinia*, inhibition at 2.0 ppm Pb by 5.44 % (0.747 mg/g) 40.76 % (0.539mg/g) and 72.44% (0.534 mg/g) in *Spirodela* respectively at 4,8 & 12 days of exposure compared to control. Two way ANOVA represents biochemical toxicity to the test plants, the concentrations were significant at p > 0.01 level but duration is not significant (Table 3 & 4).

Table 3 Two way ANOVA for biochemical effects of Lead on *Salvinia molesta*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	20.420**	7.153**	46.149**
F- value (between duration)	0.449	0.805	1.732

** Significant at P < 0.01 level

Table 4 Two way ANOVA for biochemical effects of Lead on *Spriodela polyrhiza*

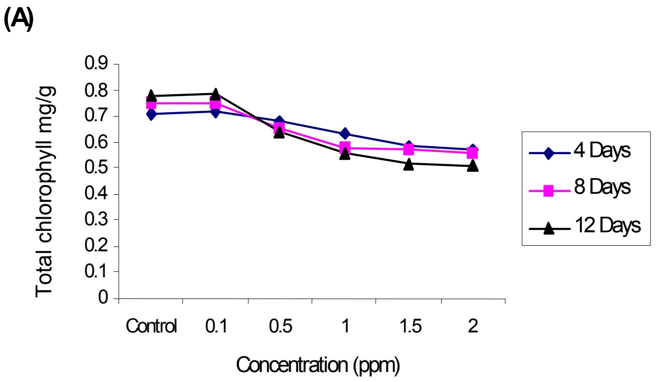
	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	4.352**	6.966**	11.91**
F- value (between duration)	0.239	0.982	6.67

** Significant at P < 0.01 level

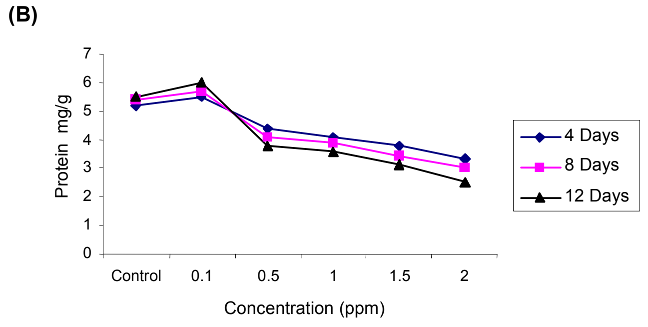
However, higher concentration (0.5, 1.0, 1.5 & 2.0 ppm) of Pb was found to inhibit chlorophyll synthesis. The inhibition of chlorophyll at higher concentration (2.0 ppm) of Pb by 34.79 % in *Salvinia*,& 72.44 % in *Spirodela* at 12 days exposure compared to their respective control.

The decline in chlorophyll content in plants exposed to Pb due to i) inhibition of important enzymes associated with chlorophyll biosynthesis ii) peroxidation of chloroplast membranes from heavy metal induced oxidative stress and iii) formation of metal stimulated chlorophyll (23). This inhibition activity of Pb is due to inhibition of haemobiosynthesis and formation of chlorophyll by integrating with functional –SH group of enzyme involved in the biosynthesis of chlorophyll (24). Similar observation was made by Singh (25) in *Hydrilla verticillata* at higher concentration of Pb at 2.0 ppm and 0.5 ppm of Cadmium. The presence of Pb decreases chlorophyll and caretonoids in *Brassica rapanus* (26). Similarly the synthesis and level of chlorophyll decreased in other plant species under the influence of Pb and Cd (27). The total chlorophyll content of experimental plants at higher concentration significantly decreased with respect to exposure duration.

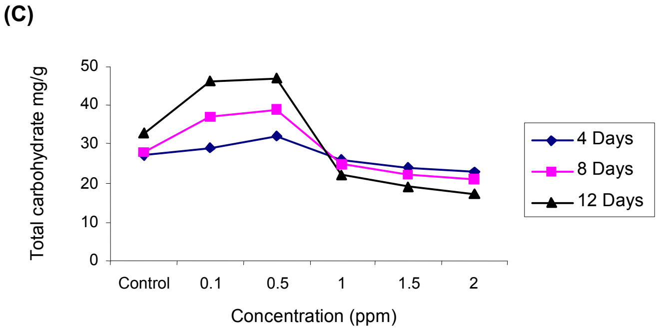
Carbohydrates acts as osmoregulators which maintains water balance in plants (28). Lower concentration (0.1 ppm) of Pb increases carbohydrate content from 7.40 % (29.0 mg/g) 32.14 % (37.0mg/g) and 39.39 % (46.0 mg/g) in *Salvinia*, and 3.22% (32.0mg/g) 26.47 % (43mg/g) and 33.33% (53.0mg/g) in *Spirodela* at 4,8 and 12 days exposure duration compared to control. Thus the percent enhancement of carbohydrate at 12 days exposure is 39.39 % in *Salvinia*, & 39.33 % in *Spirodela* However, the higher concentration of Pb inhibits the synthesis of carbohydrate and was vary from 23 mg/g to 17 mg/g in *Salvinia* 26 mg/g to 18 mg/g in *Spirodela* at 4 and 12 days exposure. The reduction in carbohydrate content can be attributed to the reduced rates of photochemical activities (14) and also Succinate Dehydrogenase (SDH) fall in cells indicate oxygen stress and energy crisis and mitochondrial disturbances (29). Generally heavy metals damages the photosynthesis apparatus in particular the harvesting complex II (23) and photosynthesis I & II (27) (Fig. 1 & 2). The protein synthesis at 0.1 ppm of Pb was promotive irrespective exposure duration in the test plants. However, the protein content was decreased at subsequent concentrations and inhibition was also directly proportional to the exposure duration also.



(A) Total Chlorophyll



(B) Carbohydrate

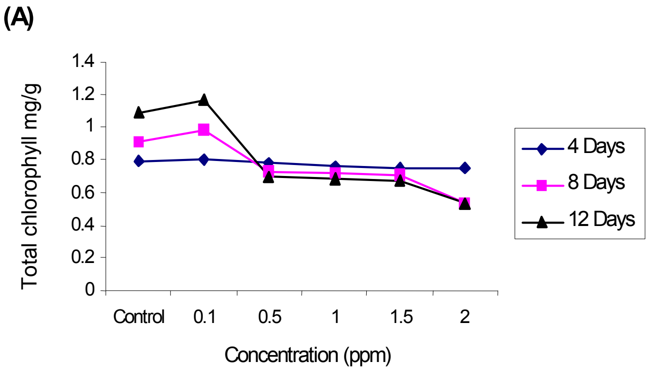


(C) Protein

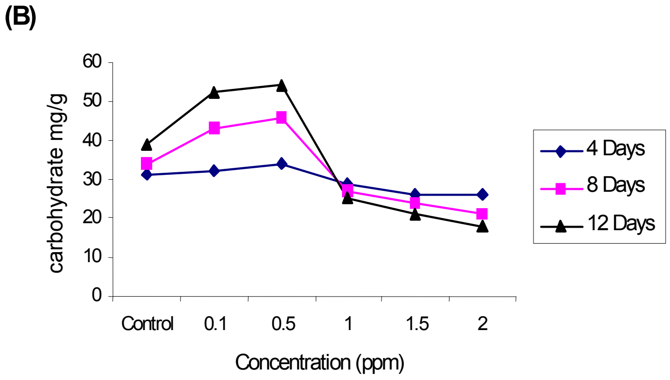
Fig 1 Biochemical effects of Lead on *Salvinia molesta*

The 0.1 ppm of Pb promoted the protein synthesis by 5.76 % (5.5 mg/g), 5.46 % (5.7mg/g) and 9.09% (6.0 mg/g) in *Salvinia*, 6.30% (8.4 mg/g), 11.11 % (9.0mg/g) and 15.2 % (14.4 mg/g) *Spirodela* at 4,8 and 12 days exposure duration respectively compared to control. The stimulation of protein synthesis at lower concentration of Pb may be altered to the synthesis of stress proteins (30). The phytochelatins (PCs) are produced by Glutathione Reductase (GR) and Phytochelatin Synthetase (PS). These proteins bind and regulate the Pb and sequesters the Pb toxicity and the plants shows the metal tolerance (31).

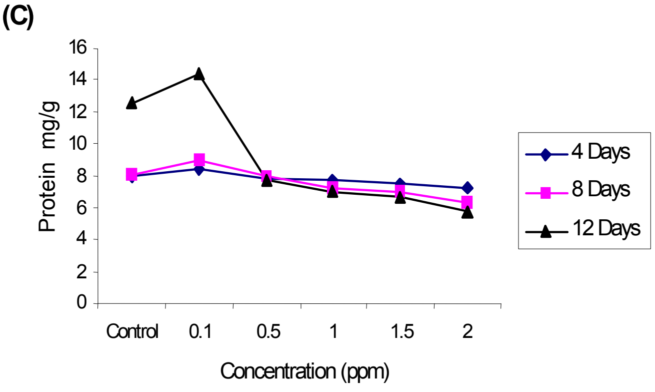
However, our investigation revealed that higher concentration of 'Pb' inhibit protein metabolism in experimental plants. The inhibition of protein content increase 36.53 % (3.3 mg/g), 44.44 % (3.0mg/g) and 54.54 % (2.5 mg/g) in *Salvinia* and 8.86 % (7.2 mg/g), 22.22% (6.3mg/g) and 53.6 % (5.8 mg/g) in *Spirodela* was noticed at 4,8 and 12 days exposure. The Cd shows slight inhibitory effect at 0.5 ppm and severe inhibition of algal growth at higher concentration in some algae (32). The DNA and RNA were inhibited, rather due to blocking of –SH group or to the inactivity of RNA and DNA polymerase activity (32) (Fig. 1 & 2).



(A) Total Chlorophyll



(B) Carbohydrate



(C) Protein

Fig 2 Biochemical effects of Lead on *Spirodela polyrhiza*

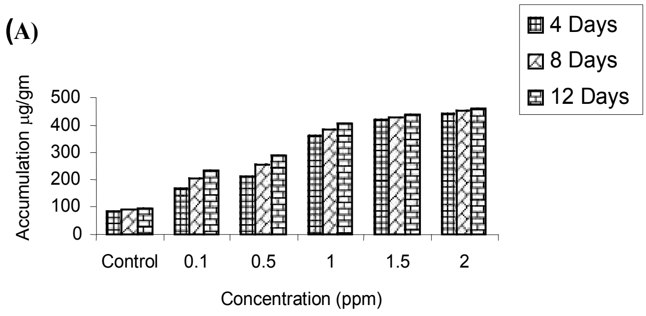
Application of two-way ANOVA is found that the biochemical responses of test plants species with respect to their concentrations were significant at $p > 0.01$ level. however, the exposure durations are not statistically significant (Table 3 & 4).

Profile of Metal Accumulation

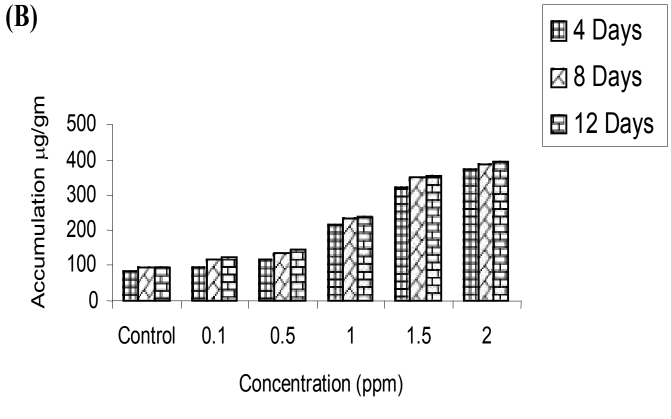
Heavy metal pollution of water is a major environmental concern, is increasing at alarming rate due to anthropogenic activities and is drawing attention and gaining paramanual importance due to its obvious impact on health through the food chain (1,33).

Fig. (3) shows the concentration of Pb accumulation in *Salvinia*,& *Spirodela*. The *Salvinia* grown in experimental pond containing 0.1 ppm found to accumulate 168 µg/g, 205 µg/g, and 231 µg/g and in *Spirodela* it is about 96 µg/g, 114 µg/g and 123 µg/g at 4,8 and 12 days exposure duration respectively. Generally in our experiments it was found that the rate of accumulation is maximum at 4 days exposure irrespective of concentrations and exposure duration, however, at subsequent concentrations and exposure durations it is marginal. Similar observations were also made by Aslam (34), in *Nastutium officinate* and *Mentha aquatica* to the exposure concentrations of 0.1 and 0.5 ppm of Cd. Similar observation was made by Sinha & Pandey (35) in the accumulation of Ni in *Hydrilla verticillata* and Cd and Pb in *Salvinia cuculata*. The increase in the accumulation might be due to increased number of binding sites for the completion of number of heavy metal ions leading to the increased absorption. Brenda (36) was also observed dramatic uptake of Zn in *Cladophora glomerata* within first minutes.

However, the higher concentration (2.0 ppm) of Pb accumulation in *Salvinia* by 443 µg/g,458 /g and 460 µg/g and in *Spirodela* by 374 µg/g , 391 µg/g and 395 µg/g during 4,8 and 12 days exposure duration respectively. The increase in the accumulation might be due to increased number of binding sites for the complexation of heavy metal ions, leading to the increased observation, however, slow accumulation may be due to binding ions to the plants and establishment of equilibrium status between adsorbate and adsorbant (33,37,38).



(A) ***Salvinia***



(B) ***Spirodela***

Fig 3 Accumulation profile of Lead by aquatic macrophytes

Generally (39, 40) reported that the accumulation of metal by aquatic macrophytes under controlled laboratory condition was dependent on metal concentration in the water. Generally it was found that plants exposed to concentration of 0.1 ppm of Pb found to accumulate maximum in *Salvinia* (23 µg/g), *Sporodela* (123 µg/g) during 12 days exposure duration followed by *Salvinia*. Similarly at high concentration of 2.0 ppm Pb *Salvinia* accumulates maximum of Pb (460 µg/g) followed by *Spirodela* (395 µg/g) during 12 days exposure duration (Fig. 3).

The initial increase in the accumulation by macrophytes may be due to increased number of binding sites for the complexation of heavy metal ions leading to the increased absorption. However, slow removal beyond an optimum dose may be attributed to the binding of almost all ions to the plants and the establishment of equilibrium between adsorbate and adsoibant at the existing operating conditions (38).

The *Spirodela* is found to be a suitable candidate for toxicity evaluation. The *Salvinia* is the most tolerant species and can be used for the remediation of heavy metals from the aquastic ecosystem and environmental monitoring.

Two-way ANOVA showed that both concentration and exposure duration were significant at $p < 0.01$ level in test plants and further Dunet's test was also applied for multiple comparison between control and different concentration treatments of test plants. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table. 5).

Table 5 Two way ANOVA with Dunet's test for multiple comparison for accumulation of Lead by aquatic macrophytes

	Salvinia	Spirodela
F-Value (between concentration)	376.56**	2558.17**
F- value (between duration)	13.54**	45.74**
Dunet's Value	20.54	6.87
Control V/s 0.1ppm	112.66	21.33
Control V/s 0.5ppm	162.33	40.33
Control V/s 1.0ppm	294.00	141.00
Control V/s 1.5ppm	342.00	251.00
Control V/s 2.0ppm	365.00	297.00

** Significant at $P < 0.01$ level

Acknowledgement

The authors are thankful to the Principal BLDEA's Degree College Jamkhandi. INDIA, Research and Development Centre, Bharthiar University Coimbatore and JSS College Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in the references of this manuscript. The authors are also grateful to editors, publishers of all those articles, journals and books from where the literature of this article has been received and discussed

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How to cite this article:

Rolli.N.M et al.2019, Toxicity Evaluation of Lead In Aquatic Macrophytes. *Int J Recent Sci Res.* 10(12), pp. 36285-36291. DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4895

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CODEN: IJRSFP (USA)

International Journal of Recent Scientific Research
Vol. 10, Issue, 12(A), pp. 36285-36291, December, 2019

ISSN: 0976-3031

International Journal of Recent Scientific Research

DOI: 10.24327/IJRSR

Research Article

TOXICITY EVALUATION OF LEAD IN AQUATIC MACROPHYTES

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DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4895

ARTICLE INFO

Article History:

Received 4th September, 2019
Received in revised form 25th October, 2019
Accepted 23rd November, 2019
Published online 28th December, 2019

Key Words:

Toxicity, Lead, Aquatic plants, Accumulation, Biochemical parameters, Symptoms.

ABSTRACT

The present study was focused on Lead (Pb) toxicity on macrophytes and biochemical parameters and profile of metal accumulation in aquatic macrophytes. The laboratory experiments were conducted for the assessment of Morphological Index Parameters (MIP), biochemical parameters and accumulation status of lead (Pb) in test plants at various concentrations, viz, 0.1, 0.5, 1.0, 1.5 and 2.0 ppm at regular interval for 12 days exposure duration. The test plants viz. *Salvinia,& Spirodela* were used for toxicity evaluation and profile of metal accumulation (Lead-Pb) from synthetic medium. The test plants were cultured in a modified Hoagland solution supplemented with $Pb(NO_3)_2$. The test plants shows visible symptoms like withering of roots, chlorosis, necrosis etc. particularly at higher concentrations i.e 1.5 ppm and 2.0 ppm, lower leaves gets decayed. However, at lower concentration i.e 0.1 ppm shows normal growth. The estimation of total chlorophyll, protein and carbohydrate of test plants showed significant increased at lower concentration i.e 0.1 ppm and decreased with increase in exposure concentrations i.e 0.5 to 2.0 ppm. It reveals that the toxic effect was directly proportional to its concentrations and exposure duration. The accumulation status was maximum in following orders (*Salvinia* > *Spirodela*) at low and higher concentrations of lead at 4 & 12 days exposure duration. However, accumulation profile in the test plants was maximum at 4 days exposure irrespective of metal concentrations and gradually decreases at subsequent exposure concentrations and duration.

INTRODUCTION

Heavy metal contamination in the water bodies is increasing at an alarming rate due to industrial and anthropogenic activities (1). Heavy metal pollution is a major environmental problem facing the modern word (1, 17). The danger of heavy metals is aggregated by their indefinite persistence in the environment because they cannot be destroyed biologically but are only transformed from oxidative state or organic complex to another. In addition, they are highly toxic for both aquatic flora and fauna (2). Heavy metals persisting in sediments may be slowly released into the water. Heavy metals viz, Zinc (Zn), Copper (Cu), Iron (Fe), Manganese (Mn)etc are represented as micronutrients (3) and are only toxic when taken in excess quantities, but nonessential ions like lead (Pb), Cadmium (Cd) and Nickel (Ni) inhibit various metabolic activities even in small quantities; (4, 5). The heavy metal lead (Pb) is selected as toxicant for the present study because it is used in several industries in India and are highly toxic to animals, humans and plants. Biological treatment of waste water through aquatic microphytes and macrophytes has great potential for its purification, which were effectively accumulates heavy metals (6). Aquatic macrophytes accumulate considerable amount of toxic metals and make the environment free from the xenobiotics. Thus, they play a significant role in cleaning up of environment and make it free from toxic pollutants. The metal tolerance of plants may be attributed to different enzymes, stress proteins and phytochelatins (7). Accumulation of metal at higher concentration causes retardation of biochemical activities and also generation of -SH group containing enzymes (8).

In the present investigation *Salvinia* and *Spirodela* common aquatic floating macrophytes, are used to study the effect of different concentrations of lead on morphology, biochemical constituents and efficiency in the accumulation of lead from the experimental pond under laboratory conditions.

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MATERIALS AND METHODS

Salvinia and *Spirodela* free floating aquatic plants from unpolluted water bodies is maintained in cement pots (1m diameter) under natural conditions at a temperature (28-30^{0}C). About 20g of young healthy *Salvinia,& Spirodela* were acclimatized for two weeks in Hoagland nutrient dolution maintaining pH between 7.1 to 7.4. The concentrations of lead in the polluted water are in the range of 0.1, 0.5, 1.0, 1.5 & 2.0 mg/l and tap water as a control. Morphological Index Parameter (MIP) viz, root length, leaf breadth and length were observed for 12 days at interval of 4 days. Photographs of test plants were taken by using Canon's Power Shot G$_2$ digital camera. For the further study the plants were harvested at the end of 4, 8 &12 days exposure and are thoroughly washed with distilled water and used for the estimation of total chlorophyll, protein and carbohydrates and also for morphological observations. Plants were harvested after 48 hours were dried at 80^{0}C for two days for metal extraction.

The fresh test plant samples of 1 g is macerated in 100 ml of 80% (v/v) chilled acetone by using pestle and mortar. The centrifuged and supernatant was used for the estimation of total chlorophyll by standard method (9) using 652 nm against the solvent (80% acetone as a blank). The protein was estimated by Lowry's method (10) using Bovine Serum Albumin (BSA) as a standard, using 660 nm and carbohydrates by phenol sulphuric acid method (11) using glucose as standard at 490 nm. Morphological characters were identified with the help of photographs, using Canon's Power Shot G$_2$ – digital camera.

The estimation of metal Pb in the test plant was carried out by using standard method (12). The dried and powdered 1 g plant material was digested by using mixed acid digestion method in Gerhardt digestion unit. The digested samples were diluted with double distilled water and filtered through Whatman filter paper No-14. The estimation of Pb was done by AAS (GBC 932 Plus Austrelia) with air acetylene oxidising flame and metal hollow cathode lamp at 217.00 nm wavelength. Working standards (SISCOP-Chem-Bombay Lab) were used for the calibration of instrument.

Statistical analysis

Data are presented as mean values ± SE from two independent experiments with three replicates each. Data were subjected to Two – way ANOVA to know significance between concentrations and between exposure duration for the accumulation of heavy metal (Pb). Further, Dunet's test is also applied for multiple comparisons between control and other concentrations. Two – way ANOVA test is also extended to know the significance between concentrations and duration for biochemical parameters.

RESULTS AND DISCUSSION

Toxic effect of lead on Morphology

Morphometric assay is one of the quantitative tool for the assessment of toxicants on test plants was measured using Morphological Index Parameters (MIP). In test plants the rate of inhibition of growth in root and leaf is directly proportional to the concentration and exposure duration of lead.

The test plants showed luxuriant growth and was observed that slight increase in the laminal length and breadth at lower concentration (0.01 ppm) in test plants. In *Salvinia* at 0.1 ppm the lead was found to promote laminal length 1.633 ± 0.072, 1.766 ± 0.027, 1.933 ± 0.027, and breadth 1.833 ± 0.072, 1.900 ± 0.047, 2.00 ± 0.081 at 4, 8 and 12 days exposure. Similarly root length 4.33 ± 0.196, 4.566 ± 0.098, 4.666 ± 0.98 at 4, 8 and 12 days exposure in *Salvinia* at 0.1 ppm concentration. In *Spirodela* at 0.1 ppm Pb was found to promote laminal length 0.800 ± 0.047, 0.866 ± 0.027, 0.933 ± 0.027 and breadth 0.600 ±0.047, 0.633 ± 0.054, 0.933 ± 0.027 at 4,8 & 12 day exposure similarly root length 2.133 ± 0.072 and 2.300 ± 0.081 at 4 & 12 days exposure (Table. 1 & 2).

However, the higher concentration of Pb at 0.5 & 2.0 ppm exhibited toxicity symptoms like chlorosis, necrosis and fall of leaves was observed particularly at 2.0 ppm the roots gets wither away.

In *Salvinia* at 2.0 ppm Pb has severely inhibit the laminal length by 1.433 ± 0.047,1.300 ± 0.024, 0.966 ± 0.072 and breadth 1.400 ± 0.047, 1.166 ± 0.027, 0.933 ± 0.072 at 4, 8 & 12 days exposure. Similarly root length inhibition 3.366 ± 0.072, 2.300 ± 0.205 at 4 & 12 days exposure.

The test plants showed normal growth at their respective lower concentration i.e 0.1 ppm. Similar observations were made in *Limnentherum cristatum* at 1.0 ppm concentration of Pb, Zn and Cr (13) confirmed root elongation of test plants at lower concentrations of Cd in some members of *Lemnaceae.* However, the heavy metals induces morphological abnormalities in algae also (14). Similar observation is found in the laminal length of *Spirodela* at 2.0 ppm by 0.500 ± 0.00, 0.300 ± 0.00 at 4 &12 days of exposure duration and breadth to 0.466 ± 0.027 & 0.300 ± 0.00 at 4 & 12days of exposure duration. Root growth inhibition to 0.800 ± 0.047 & 0.666 ± 0.054 at 4 & 12 days of exposure duration (Table. 1 & 2).

Generally the rate of inhibition in root and leaf is directly proportional to the concentration of Pb in the test plants. Two way ANOVA test states that the concentrations are significantly toxic at 5% level but duration is not significant. MCA test also represents the maximum deviation at its higher concentration compared to control. The higher concentration of lead (0.5 – 2.0 ppm) exhibited toxicity symptoms like leaf fall, chlorosis etc. were observed. Our results of toxicity symptoms of Pb at high concentrations observed were similar to (15,16**)** and also in *Salvinia natanus* (17). The decrease in root is due to partial root damage due to some enzyme systems (18). Axtell (19) reported that absorption of lead by *Lemna minor* and the effect of Pb on tissues at higher concentrations.

Toxic effect of Pb on Biochemical Parameters

A number of heavy metals required by plants as a micronutrients and they act as a part of prosthetic groups and involved in a wide variety of metabolic activities. but higher concentration of heavy metals are toxic and induces physiological and genetical impairments in plants (20).

The total chlorophyll content was very sensitive to Pb toxicity. The results found that lead at 0.1 ppm found to augment chlorophyll synthesis and was directly proportional to concentration of synthetic medium and exposure duration in the test plants. In *Salvinia* the chlorophyll content was increased by 0.56% (0.712 mg/g), 0.66% (0.752mg/g) and 0.77% (0.782 mg/g) at 4 ,8 and 12 days exposure duration. In *Spirodela* the

chlorophyll content was increased by 1.39% (0.801 mg/g), 4.61 % (0.982 mg/g) and 6.39 % (1.164 mg/g) at 4,8 and 12 days of exposure duration respectively (Table 1 & 2).

Table 1 Effect of Lead on morphology of *Salvinia molesta*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control	3.833 ± 0.072	3.9 ± 0.355	3.966 ± 0.259	1.66 ± 0.0272	1.8 ± 0.094	1.7 ± 0.094	1.833 ± 0.072	1.733 ± 0.072	1.900 ± 0.047
0.1	4.333 ± 0.196	4.566 ± 0.098	4.666 ± 0.098	1.633 ± 0.072	1.833 ± 0.072	1.766 ± 0.027	1.900 ± 0.047	1.933 ± 0.027	2.000 ± 0.081
0.5	4.400 ± 0.309	4.300 ± 0.294	4.030 ± 0.294	1.633 ± 0.072	1.766 ± 0.072	1.633 ± 0.072	1.766 ± 0.047	1.633 ± 0.072	1.733 ± 0.027
1.0	3.966 ± 0.072	3.866 ± 0.072	3.566 ± 0.196	1.633 ± 0.072	1.733 ± 0.072	1.633 ± 0.072	1.633 ± 0.072	1.566 ± 0.027	1.333 ± 0.027
1.5	3.766 ± 0.118	3.700 ± 0.124	2.966 ± 0.241	1.500 ± 0.047	1.600 ± 0.094	1.500 ± 0.047	1.466 ± 0.027	1.366 ± 0.098	1.166 ± 0.072
2.0	3.366 ± 0.072	3.066 ± 0.027	2.3 ± 0.205	1.433 ± 0.047	1.4 ± 0.047	1.300 ± 0.124	1.166 ± 0.720	0.966 ± 0.072	0.933 ± 0.072

Values are expressed in cms
Mean values ± Standard Error

Table 2 Effect of Lead on morphology of *Spirodela polyrhiza*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
				Leaf size					
	Root length			Length	Breadth	Length	Breadth	Length	Breadth
Control 0	1.946 ± 0.124	1.9 ± 0.124	1.91 ± 0.124	0.633 ± 0.054	0.466 ± 0.027	0.633 ± 0.054	0.500 ± 0.047	0.630 ± 0.054	0.566 ± 0.027
0.1	2.133 ± 0.072	2.166 ± 0.098	2.300 ± 0.081	0.800 ± 0.047	0.600 ± 0.047	0.866 ± 0.027	0.633 ± 0.054	0.933 ± 0.027	0.666 ± 0.027
0.5	1.900 ± 0.081	1.766 ± 0.027	1.633 ± 0.098	0.633 ± 0.054	0.566 ± 0.027	0.633 ± 0.054	0.533 ± 0.027	0.633 ± 0.054	0.500 ± 0.047
1.0	1.500 ± 0.235	1.400 ± 0.188	1.266± 0.108	0.566 ± 0.027	0.500 ± 0.047	0.500 ± 0.047	0.500 ± 0.047	0.500 ± 0.047	0.466 ± 0.027
1.5	1.033 ± 0.072	0.900 ± 0.00	0.833 ± 0.027	0.533 ± 0.027	0.466 ± 0.027	0.466 ± 0.027	0.40 ± 0.00	0.433 ± 0.027	0.333 ± 0.027
2.0	0.800 ± 0.047	0.766 ± 0.027	0.666 ± 0.054	0.500 ± 0.00	0.466 ± 0.027	0.466 ± 0.027	0.366 ± 0.027	0.300 ± 0.00	0.300 ± 0.00

Values are expressed in cms
Mean values ± Standard Error

The stimulation of chlorophyll synthesis may be due to phytochelatins (PCs) which play important role in detoxification of Pb (21). Phytochelatins also important role in cellular metal ion in homeostasis and detoxification (22).

However, the higher concentration of Pb found to inhibit the chlorophyll synthesis in the test plant. The inhibition at 2.0 ppm of Pb 19.13 % (0.569 mg/g) 25.70 % (0.555mg/g) and 34.79 % (0.506 mg/g) significant at $p > 0.95\%$ in *Salvinia*, inhibition at 2.0 ppm Pb by 5.44 % (0.747 mg/g) 40.76 % (0.539mg/g) and 72.44% (0.534 mg/g) in *Spirodela* respectively at 4,8 & 12 days of exposure compared to control. Two way ANOVA represents biochemical toxicity to the test plants, the concentrations were significant at $p > 0.01$ level but duration is not significant (Table 3 & 4).

Table 3 Two way ANOVA for biochemical effects of Lead on *Salvinia molesta*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	20.420**	7.153**	46.149**
F- value (between duration)	0.449	0.805	1.732

** Significant at $P < 0.01$ level

Table 4 Two way ANOVA for biochemical effects of Lead on *Spriodela polyrhiza*

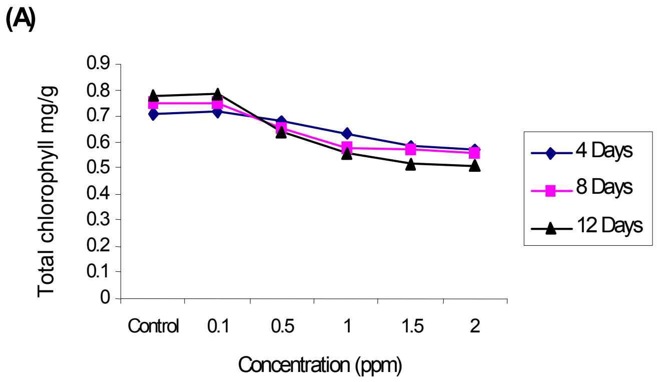
	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	4.352**	6.966**	11.91**
F- value (between duration)	0.239	0.982	6.67

** Significant at $P < 0.01$ level

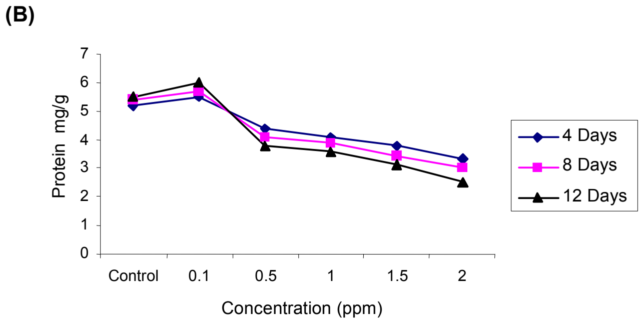
However, higher concentration (0.5, 1.0, 1.5 & 2.0 ppm) of Pb was found to inhibit chlorophyll synthesis. The inhibition of chlorophyll at higher concentration (2.0 ppm) of Pb by 34.79 % in *Salvinia*,& 72.44 % in *Spirodela* at 12 days exposure compared to their respective control.

The decline in chlorophyll content in plants exposed to Pb due to i) inhibition of important enzymes associated with chlorophyll biosynthesis ii) peroxidation of chloroplast membranes from heavy metal induced oxidative stress and iii) formation of metal stimulated chlorophyll (23). This inhibition activity of Pb is due to inhibition of haemobiosynthesis and formation of chlorophyll by integrating with functional –SH group of enzyme involved in the biosynthesis of chlorophyll (24). Similar observation was made by Singh (25) in *Hydrilla verticillata* at higher concentration of Pb at 2.0 ppm and 0.5 ppm of Cadmium. The presence of Pb decreases chlorophyll and caretonoids in *Brassica rapanus* (26). Similarly the synthesis and level of chlorophyll decreased in other plant species under the influence of Pb and Cd (27). The total chlorophyll content of experimental plants at higher concentration significantly decreased with respect to exposure duration.

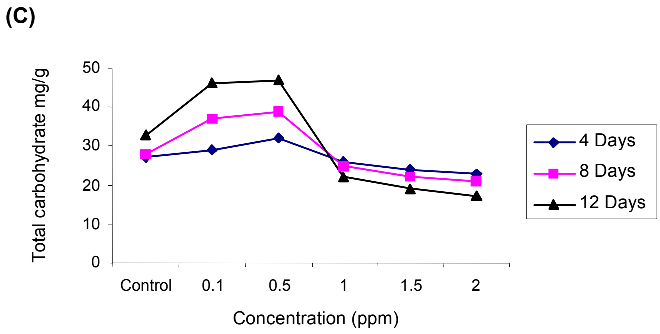
Carbohydrates acts as osmoregulators which maintains water balance in plants (28). Lower concentration (0.1 ppm) of Pb increases carbohydrate content from 7.40 % (29.0 mg/g) 32.14 % (37.0mg/g) and 39.39 % (46.0 mg/g) in *Salvinia*, and 3.22% (32.0mg/g) 26.47 % (43mg/g) and 33.33% (53.0mg/g) in *Spirodela* at 4,8 and 12 days exposure duration compared to control. Thus the percent enhancement of carbohydrate at 12 days exposure is 39.39 % in *Salvinia*, & 39.33 % in *Spirodela* However, the higher concentration of Pb inhibits the synthesis of carbohydrate and was vary from 23 mg/g to 17 mg/g in *Salvinia* 26 mg/g to 18 mg/g in *Spirodela* at 4 and 12 days exposure. The reduction in carbohydrate content can be attributed to the reduced rates of photochemical activities (14) and also Succinate Dehydrogenase (SDH) fall in cells indicate oxygen stress and energy crisis and mitochondrial disturbances (29). Generally heavy metals damages the photosynthesis apparatus in particular the harvesting complex II (23) and photosynthesis I & II (27) (Fig. 1 & 2). The protein synthesis at 0.1 ppm of Pb was promotive irrespective exposure duration in the test plants. However, the protein content was decreased at subsequent concentrations and inhibition was also directly proportional to the exposure duration also.



(A) Total Chlorophyll



(B) Carbohydrate

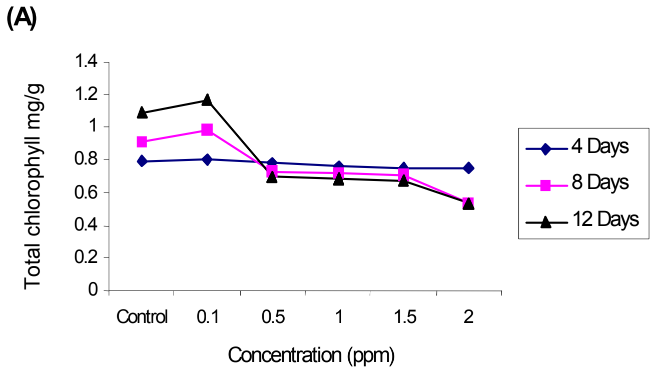


(C) Protein

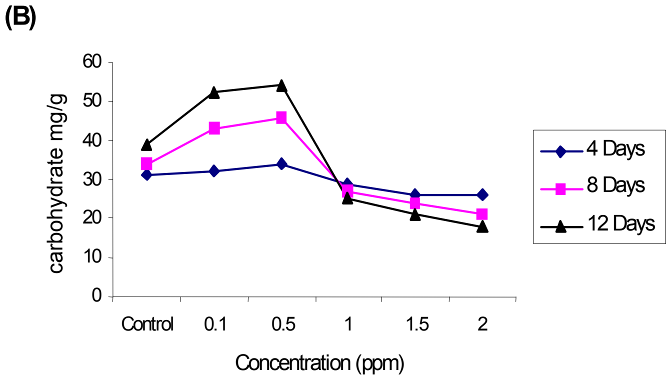
Fig 1 Biochemical effects of Lead on *Salvinia molesta*

The 0.1 ppm of Pb promoted the protein synthesis by 5.76 % (5.5 mg/g), 5.46 % (5.7mg/g) and 9.09% (6.0 mg/g) in *Salvinia*, 6.30% (8.4 mg/g), 11.11 % (9.0mg/g) and 15.2 % (14.4 mg/g) *Spirodela* at 4,8 and 12 days exposure duration respectively compared to control. The stimulation of protein synthesis at lower concentration of Pb may be altered to the synthesis of stress proteins (30). The phytochelatins (PCs) are produced by Glutathione Reductase (GR) and Phytochelatin Synthetase (PS). These proteins bind and regulate the Pb and sequesters the Pb toxicity and the plants shows the metal tolerance (31).

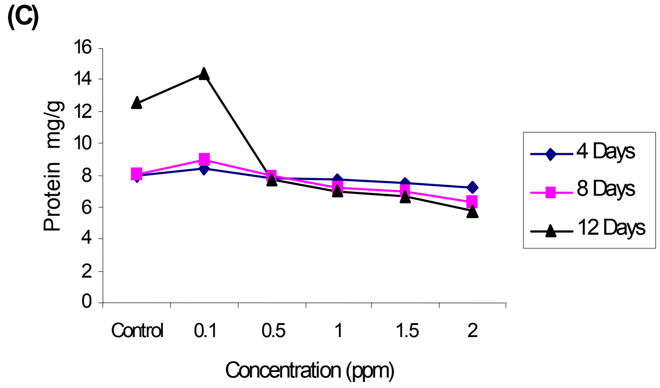
However, our investigation revealed that higher concentration of 'Pb' inhibit protein metabolism in experimental plants. The inhibition of protein content increase 36.53 % (3.3 mg/g), 44.44 % (3.0mg/g) and 54.54 % (2.5 mg/g) in *Salvinia* and 8.86 % (7.2 mg/g), 22.22% (6.3mg/g) and 53.6 % (5.8 mg/g) in *Spirodela* was noticed at 4,8 and 12 days exposure. The Cd shows slight inhibitory effect at 0.5 ppm and severe inhibition of algal growth at higher concentration in some algae (32). The DNA and RNA were inhibited, rather due to blocking of –SH group or to the inactivity of RNA and DNA polymerase activity (32) (Fig. 1 & 2).



(A) Total Chlorophyll



(B) Carbohydrate



(C) Protein

Fig 2 Biochemical effects of Lead on *Spirodela polyrhiza*

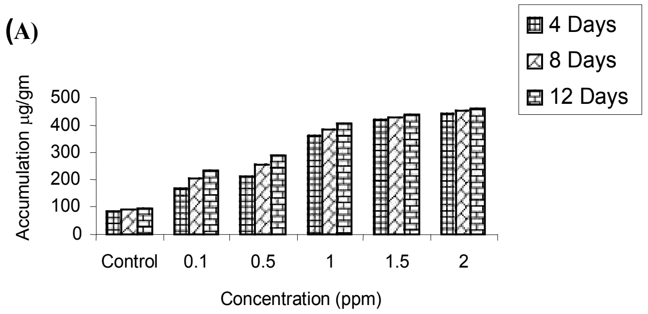
Application of two-way ANOVA is found that the biochemical responses of test plants species with respect to their concentrations were significant at $p > 0.01$ level. however, the exposure durations are not statistically significant (Table 3 & 4).

Profile of Metal Accumulation

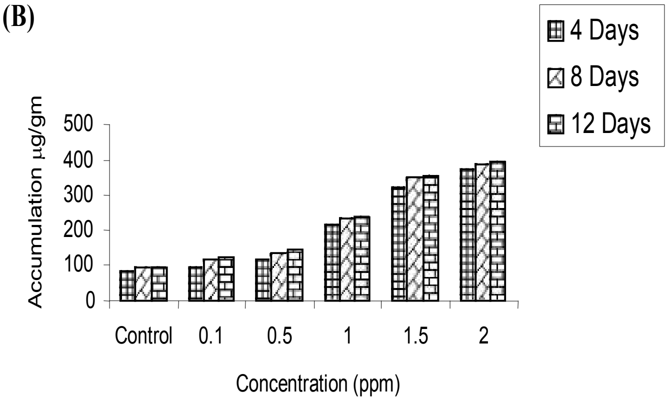
Heavy metal pollution of water is a major environmental concern, is increasing at alarming rate due to anthropogenic activities and is drawing attention and gaining paramanual importance due to its obvious impact on health through the food chain (1,33).

Fig. (3) shows the concentration of Pb accumulation in *Salvinia*,& *Spirodela*. The *Salvinia* grown in experimental pond containing 0.1 ppm found to accumulate 168 µg/g, 205 µg/g, and 231 µg/g and in *Spirodela* it is about 96 µg/g, 114 µg/g and 123 µg/g at 4,8 and 12 days exposure duration respectively. Generally in our experiments it was found that the rate of accumulation is maximum at 4 days exposure irrespective of concentrations and exposure duration, however, at subsequent concentrations and exposure durations it is marginal. Similar observations were also made by Aslam (34), in *Nastutium officinate* and *Mentha aquatica* to the exposure concentrations of 0.1 and 0.5 ppm of Cd. Similar observation was made by Sinha & Pandey (35) in the accumulation of Ni in *Hydrilla verticillata* and Cd and Pb in *Salvinia cuculata*. The increase in the accumulation might be due to increased number of binding sites for the completion of number of heavy metal ions leading to the increased absorption. Brenda (36) was also observed dramatic uptake of Zn in *Cladophora glomerata* within first minutes.

However, the higher concentration (2.0 ppm) of Pb accumulation in *Salvinia* by 443 µg/g,458 /g and 460 µg/g and in *Spirodela* by 374 µg/g , 391 µg/g and 395 µg/g during 4,8 and 12 days exposure duration respectively. The increase in the accumulation might be due to increased number of binding sites for the complexation of heavy metal ions, leading to the increased observation, however, slow accumulation may be due to binding ions to the plants and establishment of equilibrium status between adsorbate and adsorbant (33,37,38).



(A) ***Salvinia***



(B) ***Spirodela***

Fig 3 Accumulation profile of Lead by aquatic macrophytes

Generally (39, 40) reported that the accumulation of metal by aquatic macrophytes under controlled laboratory condition was dependent on metal concentration in the water. Generally it was found that plants exposed to concentration of 0.1 ppm of Pb found to accumulate maximum in *Salvinia* (23 µg/g), *Sporodela* (123 µg/g) during 12 days exposure duration followed by *Salvinia*. Similarly at high concentration of 2.0 ppm Pb *Salvinia* accumulates maximum of Pb (460 µg/g) followed by *Spirodela* (395 µg/g) during 12 days exposure duration (Fig. 3).

The initial increase in the accumulation by macrophytes may be due to increased number of binding sites for the complexation of heavy metal ions leading to the increased absorption. However, slow removal beyond an optimum dose may be attributed to the binding of almost all ions to the plants and the establishment of equilibrium between adsorbate and adsoibant at the existing operating conditions (38).

The *Spirodela* is found to be a suitable candidate for toxicity evaluation. The *Salvinia* is the most tolerant species and can be used for the remediation of heavy metals from the aquastic ecosystem and environmental monitoring.

Two-way ANOVA showed that both concentration and exposure duration were significant at $p < 0.01$ level in test plants and further Dunet's test was also applied for multiple comparison between control and different concentration treatments of test plants. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table. 5).

Table 5 Two way ANOVA with Dunet's test for multiple comparison for accumulation of Lead by aquatic macrophytes

	Salvinia	Spirodela
F-Value (between concentration)	376.56**	2558.17**
F- value (between duration)	13.54**	45.74**
Dunet's Value	20.54	6.87
Control V/s 0.1ppm	112.66	21.33
Control V/s 0.5ppm	162.33	40.33
Control V/s 1.0ppm	294.00	141.00
Control V/s 1.5ppm	342.00	251.00
Control V/s 2.0ppm	365.00	297.00

** Significant at $P < 0.01$ level

Acknowledgement

The authors are thankful to the Principal BLDEA's Degree College Jamkhandi. INDIA, Research and Development Centre, Bharthiar University Coimbatore and JSS College Dharwad for providing necessary facilities to carry out research work. Further, the authors acknowledges the immense help received from the scholars whose articles are cited and included in the references of this manuscript. The authors are also grateful to editors, publishers of all those articles, journals and books from where the literature of this article has been received and discussed

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How to cite this article:

Rolli.N.M et al.2019, Toxicity Evaluation of Lead In Aquatic Macrophytes. *Int J Recent Sci Res.* 10(12), pp. 36285-36291. DOI: http://dx.doi.org/10.24327/ijrsr.2019.1012.4895

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International Journal of Scientific Research in Mathematical and Statistical Sciences **Research Paper**
Volume-5, Issue-6, pp.328-335, December (2018) **E-ISSN:** 2348-4519

On the Zagreb polynomials of transformation graphs

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Available online at: www.isroset.org

Received: 04/Dec/2018, Accepted: 26/Dec/2018, Online: 31/Dec/20188

Abstract— In the year **2009**, Fath-Tabar introduced the concept of Zagreb polynomials. The novel topological indices called Zagreb indices can be derived from these polynomials. In order to find the Zagreb polynomials of transformation graphs we introduce the concept of Zagreb co-polynomials, from which one can derive the Zagreb coindices. Further, we establish the relations connecting the Zagreb polynomials of the graph $\boldsymbol{G}$ to those of the transformation graphs.

Keywords— *Zagreb index, Zagreb polynomial, $\boldsymbol{xyz}$-Point-Line transformation graph.*

I. INTRODUCTION

In the present work, a graph $G = (V, E)$ we mean a nontrivial, finite, simple, undirected graph with n vertices and m edges. The *degree* $d_G(v)$ of a vertex v in G is the number of edges incident to it in G. The *degree* $d_G(e)$ of an edge $e = uv$ of G in $L(G)$, is given by $d_G(e) = d_G(u) + d_G(v) - 2$. The *complement* $\overline{G}$ of a graph G is a graph whose vertex set is $V(G)$ and two vertices of $\overline{G}$ are adjacent if and only if they are nonadjacent in G. Therefore, $\overline{G}$ has n vertices and $\binom{n}{2} - m$ edges. The *line graph* [15] $L(G)$ of a graph G is a graph with vertex set which is one to one correspondence with the edge set of G and two vertices of $L(G)$ are adjacent whenever the corresponding edges in G have a vertex incident in common. The *subdivision graph* [15] $S(G)$ of a graph G is a graph with the vertex set $V(S(G)) = V(G) \cup E(G)$ and two vertices of $S(G)$ are adjacent whenever they are incident in G. The *partial complement of subdivision graph* [18] $\overline{S}(G)$ of a graph G is a graph with the vertex set $V(\overline{S}(G)) = V(G) \cup E(G)$ and two vertices of $\overline{S}(G)$ are adjacent whenever they are nonincident in G.

In this paper, we denote $u \sim v$ ($u \nsim v$) for vertices u and v are adjacent (resp., nonadjacent), $e \sim f$ ($e \nsim f$) means that the edges e and f are adjacent (resp., nonadjacent) and $u \sim e$ ($u \nsim e$) means that the vertex u and an edge e are incident (resp., nonincident) in G. The vertices of $T^{xyz}(G)$ representing the vertices of G are referred to as point-vertices while the vertices of $T^{xyz}(G)$ representing the edges of G are referred to as line-vertices. For undefined notations and terminologies one can refer [15, 19].

A topological index is a numerical parameter mathematically derived from the graph structure. It is a graph invariant. The topological indices have their applications in various disciplines of science and technology. The first and second Zagreb indices are amongst the oldest and best known topological indices defined in 1972 by Gutman [12] as follows:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) \cdot d_G(v),$$

respectively. These are widely studied degree based topological indices due to their applications in chemistry, for details see [3,8,11,13,16,24]. The first Zagreb index [21] can also be expressed as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)].$$

Ashrafi et al. [1] defined the first and second Zagreb coindices as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)]$$

and

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u) \cdot d_G(v),$$

respectively.

In 2004, Milic′evic′ et al. [20] reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees.

The first and second reformulated Zagreb indices are defined, respectively, as

$$EM_1(G) = \sum_{e\in E(G)} d_G(e)^2$$

and

$$EM_2(G) = \sum_{e\sim f} d_G(e)\cdot d_G(f).$$

In [17], Hosamani et al. defined the first and second reformulated Zagreb coindices respectively as

$$\overline{EM_1}(G) = \sum_{e\nsim f} [d_G(e) + d_G(f)]$$

and

$$\overline{EM_2}(G) = \sum_{e\nsim f} d_G(e)\cdot d_G(f).$$

Considering the Zagreb indices, Fath-Tabar [10] defined first and the second *Zagreb polynomials* as

$$M_1(G,x) = \sum_{v_i,v_j\in E(G)} x^{d_G(v_i)+d_G(v_j)}, \qquad (1.1)$$

$$M_2(G,x) = \sum_{v_i,v_j\in E(G)} x^{d_G(v_i)\cdot d_G(v_j)}, \qquad (1.2)$$

and

$$M_3(G,x) = \sum_{v_i,v_j\in E(G)} x^{|d_G(v_i)-d_G(v_j)|}, \qquad (1.3)$$

respectively, where x is a variable. In addition, Shuxian [23] defined two polynomials related to the first Zagreb index as in the form

$$M_1^*(G,x) = \sum_{v_i\in V(G)} d_G(v_i)x^{d_G(v_i)} \text{ and } M_0 = \sum_{v_i\in V(G)} x^{d_G(v_i)}.$$

In [7], A. R. Bindusree et al. defined the following polynomials

$$\begin{aligned}
M_4(G,x) &= \sum_{v_i,v_j\in E(G)} x^{d_G(v_i)((d_G(v_i)+d_G(v_j))},\\
M_5(G,x) &= \sum_{v_i,v_j\in E(G)} x^{d_G(v_j)((d_G(v_i)+d_G(v_j))},\\
M_{a,b}(G,x) &= \sum_{v_i,v_j\in E(G)} x^{ad_G(v_i)+bd_G(v_j)},\\
M'_{a,b}(G,x) &= \sum_{v_i,v_j\in E(G)} x^{(d_G(v_i)+a)(d_G(v_j)+b)}.
\end{aligned}$$

In the following section, we define new graph polynomials called Zagreb co-polynomials of a graph

The rest of the paper is organized as follows: In section II, we define and study the new graph polynomials called Zgreb co-polynomials. The section III discuss the generalized xyz-point line transformation graphs. In section IV, we obtaine the Zagreb polynomials of the generalized xyz-point line transformation graphs when $z = +$.

II. ZAGREB CO-POLYNOMIALS OF A GRAPH

In this section, we define new graph polynomials called *Zagreb co-polynomials*. The first, second, and third *Zagreb co-polynomials* of a graph G are denoted and defined as,

$$\begin{aligned}
\overline{M_1}(G,x) &= \sum_{v_i,v_j\notin E(G)} x^{d_G(v_i)+d_G(v_j)},\\
\overline{M_2}(G,x) &= \sum_{v_i,v_j\notin E(G)} x^{d_G(v_i)\cdot d_G(v_j)}
\end{aligned}$$

and

$$\overline{M_3}(G,x) = \sum_{v_i,v_j\notin E(G)} x^{|d_G(v_i)-d_G(v_j)|},$$

respectively, where x is a variable.
In addition, we define

$$\begin{aligned}
\overline{M_4}(G,x) &= \sum_{v_i,v_j\notin E(G)} x^{d_G(v_i)((d_G(v_i)+d_G(v_j))},\\
\overline{M_5}(G,x) &= \sum_{v_i,v_j\notin E(G)} x^{d_G(v_j)((d_G(v_i)+d_G(v_j))},\\
\overline{M}_{a,b}(G,x) &= \sum_{v_i,v_j\notin E(G)} x^{ad_G(v_i)+bd_G(v_j)},\\
\overline{M'}_{a,b}(G,x) &= \sum_{v_i,v_j\notin E(G)} x^{(d_G(v_i)+a)(d_G(v_j)+b)}.
\end{aligned}$$

Example 2.1. *If $G = K_2\cdot K_3$ is a graph, then the Zagreb co-polynomials of G are as follows:*

$$\overline{M_1}(G,x) = 2x^3,\quad \overline{M_2}(G,x) = 2x^2,\quad \overline{M_3}(G,x) = 2x.$$

Example 2.2. *If C_4 is a cycle of order 4, then the Zagreb co-polynomials of C_4 are as follows:*

$$\overline{M_1}(C_4,x) = 2x^4,\quad \overline{M_2}(C_4,x) = 2x^4,\quad \overline{M_3}(C_4,x) = 2.$$

Remark 2.3. *For the self-complementary graphs the Zagreb polynomials and the Zagreb co-polynomials are always same.*

Proposition 2.4. *The Zagreb co-polynomials of a path, a cycle, a complete graph, a complete bipartite graph and a wheel are as follows:*

(i) For a path P_n of order n, we have

$$\begin{aligned}
\overline{M_1}(P_n,x) &= \frac{(n^2-7n+12)}{2}x^4 + 2(n-3)x^3 + x^2,\\
\overline{M_2}(P_n,x) &= \frac{(n^2-7n+12)}{2}x^4 + 2(n-3)x^2 + x,\\
\overline{M_3}(P_n,x) &= 2(n-3)x + \frac{(n^2-7n+14)}{2}.
\end{aligned}$$

(ii) For a cycle C_n of order n, we have

$$\overline{M_1}(C_n,x) = \frac{n(n-3)}{2}x^4,\quad \overline{M_2}(C_n,x) = \frac{n(n-3)}{2}x^4$$

$$and\ \overline{M_3}(C_n,x) = \frac{n(n-3)}{2}.$$

(iii) For a complete graph of order n, we have

$$\overline{M_i}(K_n,x) = 0,\quad for\quad i = 1,2,3.$$

(iv) For a complete bipartite graph $K_{a,b}$ of order $a+b$, we have

$$\overline{M_1}(K_{a,b},x) = \frac{a(a-1)}{2}x^{2b} + \frac{b(b-1)}{2}x^{2a},$$

$$\overline{M_2}(K_{a,b},x) = \frac{a(a-1)}{2}x^{b^2} + \frac{b(b-1)}{2}x^{a^2}$$

and $\overline{M_3}(K_{a,b},x) = \frac{a(a-1)}{2} + \frac{b(b-1)}{2}.$

(v) For a wheel W_n of order n, we have

$$\overline{M_1}(W_n,x) = \frac{(n^2-5n+4)}{2}x^6,$$

$$\overline{M_2}(W_n,x) = \frac{(n^2-5n+4)}{2}x^9,$$

$$\overline{M_3}(W_n,x) = \frac{(n^2-5n+4)}{2}.$$

Theorem 2.5. *For a graph G, the Zagreb polynomials of its complement $\overline{G}$ are given by*

$$M_1(\bar{G},x) = x^{2(n-1)}\,\bar{M}_{-1,-1}\,(G,x);$$

$$M_2(\bar{G},x) = \overline{M'}_{(1-n),(1-n)}(G,x);$$

$$M_3(\bar{G},x) = \overline{M_3}(G,x).$$

Proof. The proof follows from the definitions of Zagreb polynomials and the degree of a vertex in the complement of a graph.

III. GENERALIZED xyz-POINT-LINE TRANSFORMATION GRAPH $T^{xyz}(G)$

The procedure of obtaining a new graph from a given graph using adjacency (or nonadjacency) and incidence (or nonincidence) relationship between elements of a graph is known as *Graph Transformation* and the graph obtained by doing so is called a *Transformation graph*. In [2], Wu Bayoindureng et al. introduced the total transformation graphs and studied their basic properties. For a graph $G=(V,E)$, let G^0 be the graph with $V(G^0)=V(G)$ and with no edges, G^1 the complete graph with $V(G^1)=V(G)$, $G^+=G$, and $G^-=\overline{G}$. Let $\mathcal{G}$ denotes the set of simple graphs. The following graph operations depending on $x,y,z \in \{0,1,+,-\}$ induce functions $T^{xyz}\colon \mathcal{G} \to \mathcal{G}$. These operations are introduced by Deng et al. in [9]. They referred resulting graphs as xyz-transformations of G, denoted by $T^{xyz}(G)=G^{xyz}$ and studied the Laplacian characteristic polynomials and some other Laplacian parameters of xyz-transformations of an r-regular graph G. Motivated by this, Basavanagoud [4] established the basic properties of the xyz-transformation graphs by calling them as *xyz-point-line transformation graphs* by changing the notion of xyz-transformations of a graph G as $T^{xyz}(G)$ to avoid confusion between different transformations of graphs.

Definition 1 *[8] Given a graph G with vertex set $V(G)$ and edge set $E(G)$ and three variables $x,y,z \in \{0,1,+,-\}$, the graphs obtained by the operator $T^{xyz}(G)$ (xyz-point-line transformation graph $T^{xyz}(G)$) on G is the graph with vertex set $V(T^{xyz}(G))=V(G)\cup E(G)$ and the edge set $E(T^{xyz}(G))=E((G)^x)\cup E((L(G))^y)\cup E(W)$, where $W=S(G)$ if $z=+$, $W=\overline{S}(G)$ if $z=-$, W is the graph with $V(W)=V(G)\cup E(G)$ and with no edges if $z=0$ and W is the complete bipartite graph with parts $V(G)$ and $E(G)$ if $z=1$.*

Since there are 64 distinct 3 - permutations of $\{0,1,+,-\}$. Thus obtained 64 kinds of generalized *xyz-point-line transformation graphs*. There are 16 different graphs for each case when $z=0$, $z=1$, $z=+$, $z=-$. In this paper, we consider the *xyz-point-line transformation graphs* $T^{xyz}(G)$ when $z=+$. In which,

- Subdivision graph $S(G)=T^{00+}(G)$, for details see [15],
- Semitotal-point graph $T_2(G)=T^{+0+}(G)$, for details see [22],
- Semitotal-line graph $T_1(G)=T^{0++}(G)$, for details see [14],
- Total graph $T(G)=T^{+++}(G)$, for details see [15].

The Zagreb polynomials of the graph operators $S(G), T_2(G)$ and $T_1(G)$ can be found in [7].

For instance, the total graph $T(G)$ is a graph with vertex set $V(G)\cup E(G)$ and two vertices of $T(G)$ are adjacent whenever they are adjacent or incident in G. The xyz-point-line transformation graph $T^{--+}(G)$ is a graph with vertex set $V(G)\cup E(G)$ and two vertices of $T^{--+}(G)$ are adjacent whenever they are nonadjacent or incident in G.

Example 3.2. *If $G=K_2\cdot K_3$ is a graph, then G^0 be the graph with $V(G^0)=V(G)$ and with no edges, G^1 the complete graph with $V(G^1)=V(G)$, $G^+=G$, and $G^-=\overline{G}$ which are depicted in the following Figure 1:*

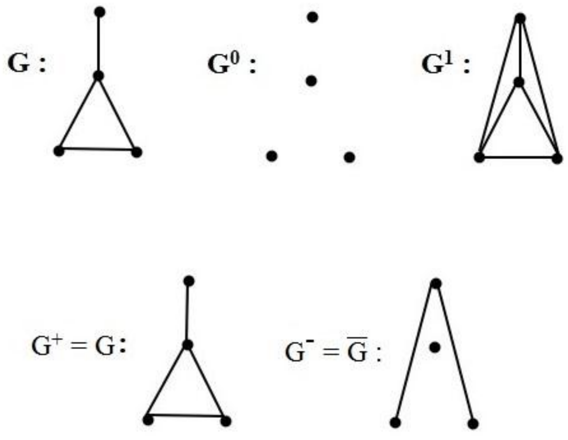

Figure 1.

The self-explanatory examples of the path P_4 and its *xyz-point-line transformation graphs* $T^{xy+}(P_4)$ are depicted in Figure 2.

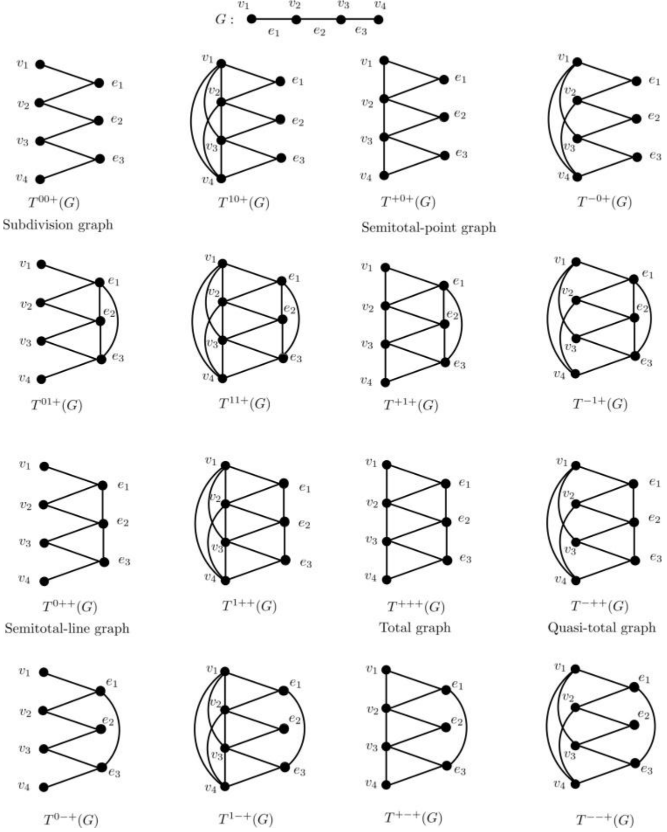

Figure 2.

IV. RESULTS ON THE ZAGREB POLYNOMIALS OF $\mathbf{T^{xy+}(G)}$

In this section, we obtain relations connecting the the *Zagreb polynomials* of a graph G and the *Zagreb polynomials* of *xyz-point-line transformation graphs* $T^{xy+}(G)$.

Let n vertices of the graph G be $v_1, v_2, \dots, v_n$, and let $e_1, e_2, \dots, e_m$ be the edges in G, where $n \geq 2$ and $m \geq 1$.

Theorem 4.1. *[5] Let G be a graph of order n, size m. Let v be the point-vertex of $T^{xy+}(G)$ and e be the line-vertex of $T^{xy+}(G)$ corresponding to a vertex v of G and to an edge e of G, respectively. Then*

$$d_{T^{xy+}(G)}(v) = \begin{cases} d_G(v) & if\ \ x = 0, y \in \{0,1,+,-\} \\ n-1+d_G(v) & if\ \ x = 1, y \in \{0,1,+,-\} \\ 2d_G(v) & if\ \ x = +, y \in \{0,1,+,-\} \\ n-1 & if\ \ x = -, y \in \{0,1,+,-\}, \end{cases}$$

$$d_{T^{xy+}(G)}(e) = \begin{cases} 2 & if\ \ x = 0, y \in \{0,1,+,-\} \\ m+1 & if\ \ x = 1, y \in \{0,1,+,-\} \\ 2+d_G(e) & if\ \ x = +, y \in \{0,1,+,-\} \\ m+1-d_G(e) & if\ \ x = -, y \in \{0,1,+,-\}. \end{cases}$$

Theorem 4.2. *For the graph $T^{11+}(G)$, the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{11+}(G),x) &= x^{2(n-1)}M_1(G,x) + x^{2(n-1)}\overline{M_1}(G,x) \\ &\quad + x^{n+m}M_1^*(G,x) + \frac{1}{2}m(m-1)x^{2(m+1)}; \\ M_2(T^{11+}(G),x) &= M'_{n-1,n-1}(G,x) + \overline{M'}_{n-1,n-1}(G,x) \\ &\quad + x^{(n-1)(m+1)}M_3(G,x) \\ &\quad + \frac{1}{2}m(m-1)x^{(m+1)^2}; \\ M_3(T^{11+}(G),x) &= M_3(G,x) + \overline{M_3}(G,x) + x^{n-m-2}M_1^*(G,x) \\ &\quad + \frac{1}{2}m(m-1). \end{aligned}$$

Proof. From Theorem 4.1, we have

$$d_{T^{11+}(G)}(v) = \begin{cases} n-1+d_G(v) & if\ \ v \in V(G), \\ m+1 & if\ \ v \in E(G). \end{cases}$$

Therefore, from Eq. (1.1), we get

$$\begin{aligned} M_1(T^{11+}(G),x) &= \sum_{uv \in E(T^{11+}(G))} x^{d_{T^{11+}(G)}(u)+d_{T^{11+}(G)}(v)} \\ &= \sum_{uv \in E(G)} x^{d_{T^{11+}(G)}(u)+d_{T^{11+}(G)}(v)} + \sum_{uv \notin E(G)} x^{d_{T^{11+}(G)}(u)+d_{T^{11+}(G)}(v)} \\ &\quad + \sum_{uv \in E(S(G))} x^{d_{T^{11+}(G)}(u)+d_{T^{11+}(G)}(v)} + \sum_{u \sim v} x^{d_{T^{11+}(G)}(u)+d_{T^{11+}(G)}(v)} \\ &= \sum_{uv \in E(G)} x^{n-1+d_G(u)+n-1+d_G(v)} + \sum_{uv \notin E(G)} x^{n-1+d_G(u)+n-1+d_G(v)} \\ &\quad + \sum_{uv \in E(S(G))} x^{n-1+d_G(u)+m+1} + \sum_{u \sim v} x^{m+1+m+1} \\ &= x^{2(n-1)}M_1(G,x) + x^{2(n-1)}\overline{M_1}(G,x) + x^{n+m} \sum_{v \in V(G)} d_G(v)x^{d_G(v)} \\ &\quad + \frac{1}{2}m(m-1)x^{2(m+1)}. \\ &= x^{2(n-1)}M_1(G,x) + x^{2(n-1)}\overline{M_1}(G,x) + x^{n+m}M_1^*(G,x) + \frac{1}{2}m(m-1)x^{2(m+1)}. \end{aligned}$$

Now, from Eq. (1.2), we get

$$\begin{aligned} M_2(T^{11+}(G),x) &= \sum_{uv \in E(T^{11+}(G))} x^{d_{T^{11+}(G)}(u) \cdot d_{T^{11+}(G)}(v)} \\ &= \sum_{uv \in E(G)} x^{d_{T^{11+}(G)}(u) \cdot d_{T^{11+}(G)}(v)} + \sum_{uv \notin E(G)} x^{d_{T^{11+}(G)}(u) \cdot d_{T^{11+}(G)}(v)} \\ &\quad + \sum_{uv \in E(S(G))} x^{d_{T^{11+}(G)}(u) \cdot d_{T^{11+}(G)}(v)} + \sum_{u \sim v} x^{d_{T^{11+}(G)}(u) \cdot d_{T^{11+}(G)}(v)} \\ &= \sum_{uv \in E(G)} x^{(n-1+d_G(u))(n-1+d_G(v))} + \sum_{uv \notin E(G)} x^{(n-1+d_G(u))(n-1+d_G(v))} \\ &\quad + \sum_{uv \in E(S(G))} x^{(n-1+d_G(u))(m+1)} + \sum_{u \sim v} x^{(m+1)(m+1)} \\ &= M'_{n-1,n-1}(G,x) + \overline{M'}_{n-1,n-1}(G,x) \\ &\quad + x^{(n-1)(m+1)}M_3(G,x^{m+1}) \\ &\quad + \frac{1}{2}m(m-1)x^{(m+1)^2} \end{aligned}$$

Finally, from Eq. (1.3), we get

$$\begin{aligned} M_3(T^{11+}(G),x) &= \sum_{uv \in E(T^{11+}(G))} x^{\left|d_{T^{11+}(G)}(u)-d_{T^{11+}(G)}(v)\right|} \\ &= \sum_{uv \in E(G)} x^{|d_{T^{11+}(G)}(u)-d_{T^{11+}(G)}(v)|} + \sum_{uv \notin E(G)} x^{|d_{T^{11+}(G)}(u)-d_{T^{11+}(G)}(v)|} \end{aligned}$$

$$\begin{aligned}
&+\sum_{uv\in E(S(G))} x^{|d_{T^{11+}(G)}(u)-d_{T^{11+}(G)}(v)|}+\sum_{u\sim v} x^{|d_{T^{11+}(G)}(u)-d_{T^{11+}(G)}(v)|}\\
=&\sum_{uv\in E(G)} x^{|n-1+d_G(u)-n+1-d_G(v)|}+\sum_{uv\notin E(G)} x^{|n-1+d_G(u)-n+1-d_G(v)|}\\
&+\sum_{uv\in E(S(G))} x^{|n-1+d_G(u)-m-1|}+\sum_{u\sim v} x^{|m+1-m-1|}\\
=&\quad M_3(G,x)+\overline{M_3}(G,x)+x^{(n-1)(m+1)}\sum_{v\in V(G)} d_G(v)x^{d_G(v)+(n-m-2)}+\frac{1}{2}m(m-1)\\
=&\quad M_3(G,x)+\overline{M_3}(G,x)+x^{(n-1)(m+1)(n-m-2)}M_1^*(G,x)+\frac{1}{2}m(m-1).
\end{aligned}$$

Theorem 4.3. *For the graph $T^{01+}(G)$, the Zagreb polynomials are given by*

$$\begin{aligned}
M_1(T^{01+}(G),x) &= x^{(m+1)}M_1^*(G,x)+\frac{1}{2}m(m-1)x^{2(m+1)};\\
M_2(T^{01+}(G),x) &= M_3(G,x^{(m+1)})+\frac{1}{2}m(m-1)x^{(m+1)^2};\\
M_3(T^{01+}(G),x) &= \frac{1}{x^{(m+1)}}M_1^*(G,x)+\frac{1}{2}m(m-1).
\end{aligned}$$

Proof. From Theorem 4.1, we get

$$d_{T^{01+}(G)}(v)=\begin{cases} d_G(v) & if\ \ v\in V(G),\\ m+1 & if\ \ v\in E(G).\end{cases}$$

Therefore, from Eq. (1.1), we get

$$\begin{aligned}
M_1(T^{01+}(G),x) &= \sum_{uv\in E(T^{01+}(G))} x^{d_{T^{01+}(G)}(u)+d_{T^{01+}(G)}(v)}\\
&= \sum_{uv\in E(S(G))} x^{d_{T^{01+}(G)}(u)+d_{T^{01+}(G)}(v)}+\sum_{u,v\in E(G)} x^{d_{T^{01+}(G)}(u)+d_{T^{01+}(G)}(v)}\\
&= \sum_{uv\in E(S(G))} x^{d_G(u)+m+1}+\sum_{u,v\in E(G)} x^{m+1+m+1}\\
&= \textstyle\sum_{v\in V(G)} d_G(v)x^{d_G(v)+(m+1)}+\frac{1}{2}m(m-1)x^{2(m+1)}\\
&= x^{(m+1)}M_1^*(G,x)+\tfrac{1}{2}m(m-1)x^{2(m+1)}.
\end{aligned}$$

Now, from Eq. (1.2), we get

$$\begin{aligned}
M_2(T^{01+}(G),x) &= \sum_{uv\in E(T^{01+}(G))} x^{d_{T^{01+}(G)}(u)\cdot d_{T^{01+}(G)}(v)}\\
&= \sum_{uv\in E(S(G))} x^{d_{T^{01+}(G)}(u)\cdot d_{T^{01+}(G)}(v)}+\sum_{u,v\in E(G)} x^{d_{T^{01+}(G)}(u)\cdot d_{T^{01+}(G)}(v)}\\
&= \sum_{uv\in E(S(G))} x^{d_G(u)(m+1)}+\sum_{u,v\in E(G)} x^{(m+1)(m+1)}\\
&= \sum_{v\in V(G)} d_G(v)x^{d_G(v)(m+1)}+\frac{1}{2}m(m-1)x^{(m+1)^2}\\
&= M_3(G,x^{(m+1)})+\frac{1}{2}m(m-1)x^{(m+1)^2}.
\end{aligned}$$

Finally, from Eq. (1.3), we get

$$\begin{aligned}
M_3(T^{01+}(G),x) &= \sum_{uv\in E(T^{01+}(G))} x^{\left|d_{T^{01+}(G)}(u)-d_{T^{01+}(G)}(v)\right|}\\
&= \sum_{uv\in E(S(G))} x^{|d_{T^{01+}(G)}(u)-d_{T^{01+}(G)}(v)|}\\
&\quad+\sum_{u,v\in E(G)} x^{|d_{T^{01+}(G)}(u)-d_{T^{01+}(G)}(v)|}\\
&= \sum_{uv\in E(S(G))} x^{|d_G(u)-m-1|}+\sum_{u,v\in E(G)} x^{|m+1-m-1|}\\
&= \sum_{v\in V(G)} d_G(v)x^{|d_G(v)-(m+1)|}+\frac{1}{2}m(m-1)\\
&= \frac{1}{x^{(m+1)}}M_1^*(G,x)+\frac{1}{2}m(m-1).
\end{aligned}$$

Theorem 4.4. *For the graph $T^{-0+}(G)$, the Zagreb polynomials are given by*

$$\begin{aligned}
M_1(T^{-0+}(G),x) &= \left(\binom{n}{2}-m\right)x^{2(n-1)}+2mx^{(n+1)};\\
M_2(T^{-0+}(G),x) &= \left(\binom{n}{2}-m\right)x^{(n-1)^2}+2mx^{2(n-1)};\\
M_3(T^{-0+}(G),x) &= \binom{n}{2}-m+2mx^{|n-3|}.
\end{aligned}$$

Proof. From Theorem 4.1, we have

$$d_{T^{-0+}(G)}(v)=\begin{cases} n-1 & if\ \ v\in V(G),\\ 2 & if\ \ v\in E(G).\end{cases}$$

Therefore, from Eq. (1.1), we get

$$\begin{aligned}
M_1(T^{-0+}(G),x) &= \sum_{uv\in E(T^{-0+}(G))} x^{d_{T^{-0+}(G)}(u)+d_{T^{-0+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{d_{T^{-0+}(G)}(u)+d_{T^{-0+}(G)}(v)}+\sum_{uv\in E(S(G))} x^{d_{T^{-0+}(G)}(u)+d_{T^{-0+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{n-1+n-1}+\sum_{uv\in E(S(G))} x^{n-1+2}\\
&= \left(\binom{n}{2}-m\right)x^{2(n-1)}+2mx^{(n+1)}.
\end{aligned}$$

Now, from Eq. (1.2), we get

$$\begin{aligned}
M_2(T^{-0+}(G),x) &= \sum_{uv\in E(T^{-0+}(G))} x^{d_{T^{-0+}(G)}(u)\cdot d_{T^{-0+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{d_{T^{-0+}(G)}(u)\cdot d_{T^{-0+}(G)}(v)}+\sum_{uv\in E(S(G))} x^{d_{T^{-0+}(G)}(u)\cdot d_{T^{-0+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{(n-1)^2}+\sum_{uv\in E(S(G))} x^{2(n-1)}\\
&= \left(\binom{n}{2}-m\right)x^{(n-1)^2}+2mx^{2(n-1)}.
\end{aligned}$$

Finally from Eq. (1.3), we get

$$\begin{aligned}
M_3(T^{-0+}(G),x) &= \sum_{uv\in E(T^{-0+}(G))} x^{|d_{T^{-0+}(G)}(u)-d_{T^{-0+}(G)}(v)|}\\
&= \sum_{uv\notin E(G)} x^{|d_{T^{-0+}(G)}(u)-d_{T^{-0+}(G)}(v)|}+\sum_{uv\in E(S(G))} x^{|d_{T^{-0+}(G)}(u)-d_{T^{-0+}(G)}(v)|}\\
&= \sum_{uv\notin E(G)} x^{|n-1-n+1|}+\sum_{uv\in E(S(G))} x^{|n-1-2|}\\
&= \binom{n}{2}-m+2mx^{|n-3|}.
\end{aligned}$$

Theorem 4.5. *For the graph $T^{-1+}(G)$, the Zagreb polynomials are given by*

$$\begin{aligned}
M_1(T^{-1+}(G),x) &= \left(\binom{n}{2}-m\right)x^{2(n-1)}+2mx^{(n+m)}+\binom{m}{2}x^{2(m+1)};\\
M_2(T^{-1+}(G),x) &= \left(\binom{n}{2}-m\right)x^{(n-1)^2}+2mx^{(n-1)(m+1)}+\binom{m}{2}x^{(m+1)^2};\\
M_3(T^{-1+}(G),x) &= \frac{1}{2}(n(n-1)-m(m+1))+2mx^{|n-m-2|}.
\end{aligned}$$

Proof. From Theorem 4.1, we have

$$d_{T^{-1+}(G)}(v)=\begin{cases} n-1 & if\ \ v\in V(G),\\ m+1 & if\ \ v\in E(G).\end{cases}$$

Therefore, from Eq. (1.1), we get

$$\begin{aligned}
M_1(T^{-1+}(G),x) &= \sum_{uv\in E(T^{-1+}(G))} x^{d_{T^{-1+}(G)}(u)+d_{T^{-1+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{d_{T^{-1+}(G)}(u)+d_{T^{-1+}(G)}(v)}+\sum_{uv\in E(S(G))} x^{d_{T^{-1+}(G)}(u)+d_{T^{-1+}(G)}(v)}\\
&\quad+\sum_{u,v\in E(G)} x^{d_{T^{-1+}(G)}(u)+d_{T^{-1+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{2(n-1)}+\sum_{uv\in E(S(G))} x^{(n+m)}+\sum_{u,v\in E(G)} x^{2(m+1)}\\
&= \left(\binom{n}{2}-m\right)x^{2(n-1)}+2mx^{(n+m)}+\binom{m}{2}x^{2(m+1)}.
\end{aligned}$$

Now, from Eq. (1.2), we get

$$\begin{aligned}
M_2(T^{-1+}(G),x) &= \sum_{uv\in E(T^{-1+}(G))} x^{d_{T^{-1+}(G)}(u)\cdot d_{T^{-1+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{d_{T^{-1+}(G)}(u)\cdot d_{T^{-1+}(G)}(v)}+\sum_{uv\in E(S(G))} x^{d_{T^{-1+}(G)}(u)\cdot d_{T^{-1+}(G)}(v)}\\
&\quad+\sum_{u,v\in E(G)} x^{d_{T^{-1+}(G)}(u)\cdot d_{T^{-1+}(G)}(v)}\\
&= \sum_{uv\notin E(G)} x^{(n-1)(n-1)}+\sum_{uv\in E(S(G))} x^{(n-1)(m+1)}+\sum_{u,v\in E(G)} x^{(m+1)(m+1)}\\
&= \left(\binom{n}{2}-m\right)x^{(n-1)^2}+2mx^{(n-1)(m+1)}+\binom{m}{2}x^{(m+1)^2}.
\end{aligned}$$

Finally, from Eq. (1.3), we get

$$\begin{aligned}
M_3(T^{-1+}(G),x) &= \sum_{uv\in E(T^{-1+}(G))} x^{|d_{T^{-1+}(G)}(u)-d_{T^{-1+}(G)}(v)|}\\
&= \sum_{uv\notin E(G)} x^{|d_{T^{-1+}(G)}(u)-d_{T^{-1+}(G)}(v)|}+\sum_{uv\in E(S(G))} x^{|d_{T^{-1+}(G)}(u)-d_{T^{-1+}(G)}(v)|}\\
&\quad+\sum_{u:v} x^{|d_{T^{-1+}(G)}(u)-d_{T^{-1+}(G)}(v)|}\\
&= \sum_{uv\notin E(G)} x^{0}+\sum_{uv\in E(S(G))} x^{|n-m-2|}+\sum_{u,v\in E(G)} x^{0}\\
&= \frac{1}{2}(n(n-1)-m(m+1))+2mx^{|n-m-2|}.
\end{aligned}$$

Theorem 4.6. *For the graph $T^{10+}(G)$, the Zagreb polynomials are given by*

$$\begin{aligned}
M_1(T^{10+}(G),x) &= x^{2(n-1)}M_1(G,x)+x^{2(n-1)}\overline{M_1}(G,x)\\
&\quad+x^{n+1}M_1^{*}(G,x);\\
M_2(T^{10+}(G),x) &= M'_{n-1,n-1}(G,x)+\overline{M'}_{n-1,n-1}(G,x)\\
&\quad+x^{2(n-1)}M_3(G,x^2);\\
M_3(T^{10+}(G),x) &= M_3(G,x)+\overline{M_3}(G,x)+x^{|n-3|}M_1^{*}(G,x).
\end{aligned}$$

Proof. From Theorem 4.1, we have

$$d_{T^{10+}(G)}(v)=\begin{cases} n-1+d_G(v) & if\ \ v\in V(G),\\ 2 & if\ \ v\in E(G).\end{cases}$$

Therefore, from Eq. (1.1), we get

$$\begin{aligned}
M_1(T^{10+}(G),x) &= \sum_{uv\in E(T^{10+}(G))} x^{d_{T^{10+}(G)}(u)+d_{T^{10+}(G)}(v)}\\
&= \sum_{uv\in E(G)} x^{d_{T^{10+}(G)}(u)+d_{T^{10+}(G)}(v)}+\sum_{uv\notin E(G)} x^{d_{T^{10+}(G)}(u)+d_{T^{10+}(G)}(v)}\\
&\quad+\sum_{uv\in E(S(G))} x^{d_{T^{10+}(G)}(u)+d_{T^{10+}(G)}(v)}\\
&= \sum_{uv\in E(G)} x^{n-1+d_G(u)+n-1+d_G(v)}+\sum_{uv\notin E(G)} x^{n-1+d_G(u)+n-1+d_G(v)}\\
&\quad+\sum_{uv\in E(S(G))} x^{n-1+d_G(u)+2}\\
&= x^{2(n-1)}M_1(G,x)+x^{2(n-1)}\overline{M_1}(G,x)+x^{(n+1)}\sum_{v\in V(G)} d_G(v)x^{d_G(v)}\\
&= x^{2(n-1)}M_1(G,x)+x^{2(n-1)}\overline{M_1}(G,x)+x^{(n+1)}M_1^{*}(G,x).
\end{aligned}$$

Now, from Eq. (1.2), we get

$$\begin{aligned}
M_2(T^{10+}(G),x) &= \sum_{uv\in E(T^{10+}(G))} x^{d_{T^{10+}(G)}(u)\cdot d_{T^{10+}(G)}(v)}\\
&= \sum_{uv\in E(G)} x^{d_{T^{10+}(G)}(u)\cdot d_{T^{10+}(G)}(v)}+\sum_{uv\notin E(G)} x^{d_{T^{10+}(G)}(u)\cdot d_{T^{10+}(G)}(v)}\\
&\quad+\sum_{uv\in E(S(G))} x^{d_{T^{10+}(G)}(u)\cdot d_{T^{10+}(G)}(v)}\\
&= \sum_{uv\in E(G)} x^{(n-1+d_G(u))(n-1+d_G(v))}+\sum_{uv\notin E(G)} x^{(n-1+d_G(u))(n-1+d_G(v))}\\
&\quad+\sum_{uv\in E(S(G))} x^{(n-1+d_G(u))(2)}\\
&= M'_{n-1,n-1}(G,x)+\overline{M'}_{n-1,n-1}(G,x)+x^{2(n-1)}\sum_{v\in V(G)} d_G(v)x^{2d_G(v)}\\
&= M'_{n-1,n-1}(G,x)+\overline{M'}_{n-1,n-1}(G,x)+x^{2(n-1)}M_3\big(G,x^2\big).
\end{aligned}$$

Finally, from Eq. (1.3), we get

$$\begin{aligned}
M_3(T^{10+}(G),x) &= \sum_{uv\in E(T^{10+}(G))} x^{|d_{T^{10+}(G)}(u)-d_{T^{10+}(G)}(v)|}\\
&= \sum_{uv\in E(G)} x^{|d_{T^{10+}(G)}(u)-d_{T^{10+}(G)}(v)|}+\sum_{uv\notin E(G)} x^{|d_{T^{10+}(G)}(u)-d_{T^{10+}(G)}(v)|}\\
&\quad+\sum_{uv\in E(S(G))} x^{|d_{T^{10+}(G)}(u)-d_{T^{10+}(G)}(v)|}\\
&= \sum_{uv\in E(G)} x^{|n-1+d_G(u)-n+1-d_G(v)|}+\sum_{uv\notin E(G)} x^{|n-1+d_G(u)-n+1-d_G(v)|}\\
&\quad+\sum_{uv\in E(S(G))} x^{|n-1+d_G(u)-2|}\\
&= M_3(G,x)+\overline{M_3}(G,x)+x^{|n-3|}M_1^{*}(G,x).
\end{aligned}$$

The proof of following theorems are analogous to that of the above theorems.

Theorem 4.7. *For the graph $T^{1-+}(G)$, the Zagreb polynomials are given by*

$$\begin{aligned}
M_1(T^{1-+}(G),x) &= x^{2(n-1)}M_1(G,x)+x^{2(n-1)}\overline{M_1}(G,x)\\
&\quad+x^{n+m}\sum_{u\sim e} x^{d_G(u)+d_G(e)}\\
&\quad+x^{-2(m+1)}\overline{M_1}(L(G),x);
\end{aligned}$$

$$\begin{aligned} M_2(T^{1-+}(G),x) &= {M'}_{n-1,n-1}(G,x) + \overline{M'}_{n-1,n-1}(G,x) \\ &+ \sum_{u\sim e} x^{(n-1+d_G(u))(m+1-d_G(e))} \\ &+ \overline{M'}_{-(m+1),-(m+1)}(L(G),x); \\ M_3(T^{1-+}(G),x) &= M_3(G,x) + \overline{M_3}(G,x) \\ &+ x^{|n-m-2|}\sum_{u\sim e} x^{|d_G(u)-d_G(e)|} \\ &+ \overline{M_3}(L(G),x). \end{aligned}$$

Theorem 4.8. *For the graph* $T^{+1+}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{+1+}(G),x) &= M_1(G,x^2) + x^{(m+1)}M_1^*(G,x^2) + \binom{m}{2}x^{2(m+1)}; \\ M_2(T^{+1+}(G),x) &= M_2(G,x^4) + M_1^*(G,x^{2(m+1)}) + \binom{m}{2}x^{(m+1)^2}; \\ M_3(T^{+1+}(G),x) &= M_3(G,x^2) + \frac{1}{x^{(m+1)}}M_1^*(G,x^2) + \binom{m}{2}. \end{aligned}$$

Theorem 4.9. *For the graph* $T^{1++}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{1++}(G),x) &= x^{2(n-1)}M_1(G,x) + x^{2(n-1)}\overline{M_1}(G,x) \\ &+ x^{n+1}\sum_{u\sim e} x^{d_G(u)+d_G(e)} + x^4M_1(L(G),x); \\ M_2(T^{1++}(G),x) &= {M'}_{n-1,n-1}(G,x) + \overline{M'}_{n-1,n-1}(G,x) \\ &+ \sum_{u\sim e} x^{(n-1+d_G(u))(2+d_G(e))} \\ &+ M_2(L(G),x^4); \\ M_3(T^{1++}(G),x) &= M_3(G,x) + \overline{M_3}(G,x) \\ &+ x^{|n-3|}\sum_{u\sim e} x^{|d_G(u)-d_G(e)|} + M_3(L(G),x). \end{aligned}$$

Theorem 4.10. *For the graph* $T^{+++}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{+++}(G),x) &= M_1(G,x^2) + M_{3,1}(G,x) \\ &+ x^4M_1(L(G),x); \\ M_2(T^{+++}(G),x) &= M_2(G,x^4) + x^2M_4(G,x) \\ &+ M'_{2,2}(L(G),x); \\ M_3(T^{+++}(G),x) &= M_3(G,x^2) + M_3(G,x) + M_3(L(G),x). \end{aligned}$$

Theorem 4.11. *For the graph* $T^{-++}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{-++}(G),x) &= \left(\binom{n}{2} - m\right)x^{2(n-1)} + x^{(n+m-2)}M_1(G,x) \\ &+ x^{-2(m+1)}M_1(L(G),x); \\ M_2(T^{-++}(G),x) &= \left(\binom{n}{2} - m\right)x^{2(n-1)} + x^{(n+m-2)}M_1(G,x) \\ &+ x^{-2(\mathrm{m}+1)}M_1(L(G),x); \\ M_3(T^{-++}(G),x) &= \left(\binom{n}{2} - m\right) + x^{n-m-4}M_1(G,x) \\ &+ M_3(L(G),x). \end{aligned}$$

Theorem 4.12. *For the graph* $T^{0-+}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{0-+}(G),x) &= x^{m+1}\sum_{u\sim e} x^{d_G(u)-d_G(e)} \\ &+ x^{2(m+1)}\overline{M_1}(L(G),x); \\ M_2(T^{0-+}(G),x) &= \sum_{u\sim e} x^{d_G(u)(m+1-d_G(e))} \\ &+ \overline{M'}_{-(m+1,-(m+1)}(G,x); \\ M_3(T^{0-+}(G),x) &= x^{|1-m|}M_1^*(G,x) + \overline{M_3}(L(G),x). \end{aligned}$$

Theorem 4.13. *For the graph* $T^{+-+}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{+-+}(G),x) &= M_1(G,x^2) + x^{(m+1)}\sum_{u\sim e} x^{2d_G(u)-d_G(e)} \\ &+ x^{-2(m+1)}\overline{M_1}(L(G),x); \\ M_2(T^{+-+}(G),x) &= M_2(G,x^4) + \sum_{u\sim e} x^{2d_G(u)(m+1-d_G(e))} \\ &+ \overline{M'}_{-(m+1),-(m+1)}(L(G),x); \\ M_3(T^{+-+}(G),x) &= M_3(G,x^2) + \sum_{u\sim e} x^{|2d_G(u)-m-1+d_G(e)|} \\ &+ \overline{M_3}(L(G),x). \end{aligned}$$

Theorem 4.14. *For the graph* $T^{--+}(G)$, *the Zagreb polynomials are given by*

$$\begin{aligned} M_1(T^{--+}(G),x) &= \left(\binom{n}{2} - m\right)x^{2(n-1)} \\ &+ 2x^{-(n+m)}M_0(L(G),x) \\ &+ x^{-2(m+1)}\overline{M_1}(L(G),x); \\ M_2(T^{--+}(G),x) &= \left(\binom{n}{2} - m\right)x^{(n-1)^2} \\ &+ x^{-(n-1)(m+1)}M_0\left(L(G),x^{(n-1)}\right) \\ &+ \overline{M}'_{-(m+1),-(m+1)}(L(G),x); \\ M_3(T^{--+}(G),x) &= \left(\binom{n}{2} - m\right) + x^{(n-m-2)}M_0(L(G),x) \\ &+ \overline{M_3}(L(G),x). \end{aligned}$$

V. CONCLUSION

In this paper, we defined a set of new graph polynomials called Zagreb co-polynomials. Further, the Zagreb polynomials of the generalized xyz-point line transformation graphs (for $z = +$) are obtained. In future, one can study the Zagreb co-polynomials of different transformation graphs.

ACKNOWLEDGEMENT

The authors are thankful to the referee for useful suggestions. The first author is thankful to University Grants Commission (UGC), Government of India, New Delhi, for the financial support through UGC-SAP DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I) dated: 29th Feb. 2016. The second author is thankful to Directorate of Minorities, Government of Karnataka, Bangalore, for the financial support through M. Phil/Ph. D. Fellowship 2017-18: No. DOM/FELLOWSHIP/CR-29/2017-18 dated: 09th Aug. 2017.

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Journal of Computer and Mathematical Sciences, *Vol.9(10),1360-1383 October 2018* *ISSN 0976-5727 (Print)*
(An International Research Journal), *www.compmath-journal.org* *ISSN 2319-8133 (Online)*

Computing Leap Zagreb Indices of Generalized xyz-Point-Line Transformation Graphs $T^{xyz}(G)$ when $z=+$

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(Received on: August 29, 2018)

ABSTRACT

For a graph G, the first, second, and third leap Zagreb indices are the sum of squares of 2-distance degree of vertices of G; the sum of product of 2-distance degree of end vertices of edges in G, and the sum of product of 1-distance degree and 2-distance degrees of vertices of G, respectively. In this paper, we obtain the expressions for these three leap Zagreb indices of generalized xyz-*point-line transformation graphs* $T^{xyz}(G)$ when $z=+$ in terms of elements of the graph G.

AMS Subject Classification: 05C07, 05C12.

Keywords: Distance, degree, diameter, Zagreb index, leap Zagreb index, reformulated Zagreb index.

1. INTRODUCTION

Throughout this paper, by a graph $G=(V,E)$ we mean a simple, connected, nontrivial, undirected and finite graph of order n and size m. The k^{th} neighborhood[19] $N_k(v/G)$ of a vertex v is the set $\{u \in V(G): d(u,v)=k\}$ and the *k-distance degree* $d_k(v/G)$ of a vertex $v \in V(G)$ is $|N_k(v/G)|$, where $d(u,v)$ is the distance between the vertices u and v in G i.e., the length of the shortest path joining u and v in G. The *eccentricity* $e(v)$ of a vertex $v \in V(G)$ is given by $e(v)=max\{d(u,v): u \in V(G)\}$. We denote, $N_1(v/G)$ by $N_G(v)$, $d_1(v/G)$ by $d_G(v)$ and $e(v)$ by $e(v/G)$.

The *line graph*[12] $L(G)$ of a graph G is a graph with vertex set which is one to one correspondence with the edge set of G and two vertices of $L(G)$ are adjacent whenever the corresponding edges in G have a vertex incident in common. The *degree* $d_1(e/G)$ (or simply $d_G(e)$) of an edge $e = uv$ of G in $L(G)$, is given by $d_1(e/G) = d_1(u/G) + d_1(v/G) - 2$. The *subdivision graph*[12] $S(G)$ of a graph G is a graph with the vertex set $V(S(G)) = V(G) \cup E(G)$ and two vertices of $S(G)$ are adjacent whenever they are incident in G. The *partial complement of subdivision graph*[14] $\overline{S}(G)$ of a graph G is a graph with the vertex set $V(\overline{S}(G)) = V(G) \cup E(G)$ and two vertices of $\overline{S}(G)$ are adjacent whenever they are nonincident in G. We follow[12,15] for unexplained graph theoretic terminology and notations. The first and second Zagreb indices[10] of a graph G are defined as follows:

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 \textit{ and } M_2(G) = \sum_{uv \in E(G)} d_G(u) \cdot d_G(v),$$

respectively. In[1] Ashrafi *et al.* defined the first and second Zagreb coindices as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d_G(u) + d_G(v)] \quad \textit{and} \quad \overline{M_2}(G) = \sum_{uv \notin E(G)} d_G(u) \cdot d_G(v),$$

respectively.

In 2004, *Milic′evic′ et al.*[16] reformulated the Zagreb indices in terms of edge-degrees instead of vertex-degrees. The first and second reformulated Zagreb indices are defined respectively as,

$$EM_1(G) = \sum_{e \in E(G)} d_G(e)^2 \quad \textit{and} \quad EM_2(G) = \sum_{e \sim f} d_G(e) \cdot d_G(f).$$

In[13], Hosamani *et al.* defined the first and second reformulated Zagreb coindices respectively as,

$$\overline{EM_1}(G) = \sum_{e \sim f} [d_G(e) + d_G(f)] \quad \textit{and} \quad \overline{EM_2}(G) = \sum_{e \nsim f} d_G(e) \cdot d_G(f).$$

Then the third, fourth and fifth Zagreb indices are defined in[4] respectively as follows:

$$M_3(G) = \sum_{uv, vw \in E(G)} d_G(v)^2, \quad M_4(G) = \sum_{uv, vw \in E(G)} [d_G(u) + 2d_G(v) + d_G(w)] \text{ and}$$

$$M_5(G) = \sum_{uv, vw \in E(G)} [d_G(u)d_G(v) + d_G(v)d_G(w) + d_G(w)d_G(u)].$$

In 2017, Naji *et al.*[17] introduced the concept of leap Zagreb indices. For a graph G, the first, second, and third leap Zagreb indices are denoted and defined respectively as,

$$LM_1(G) = \sum_{v\in V(G)} d_2(v/G)^2, \qquad (1.1)$$

$$LM_2(G) = \sum_{uv\in E(G)} d_2(u/G)\cdot d_2(v/G), \qquad (1.2)$$

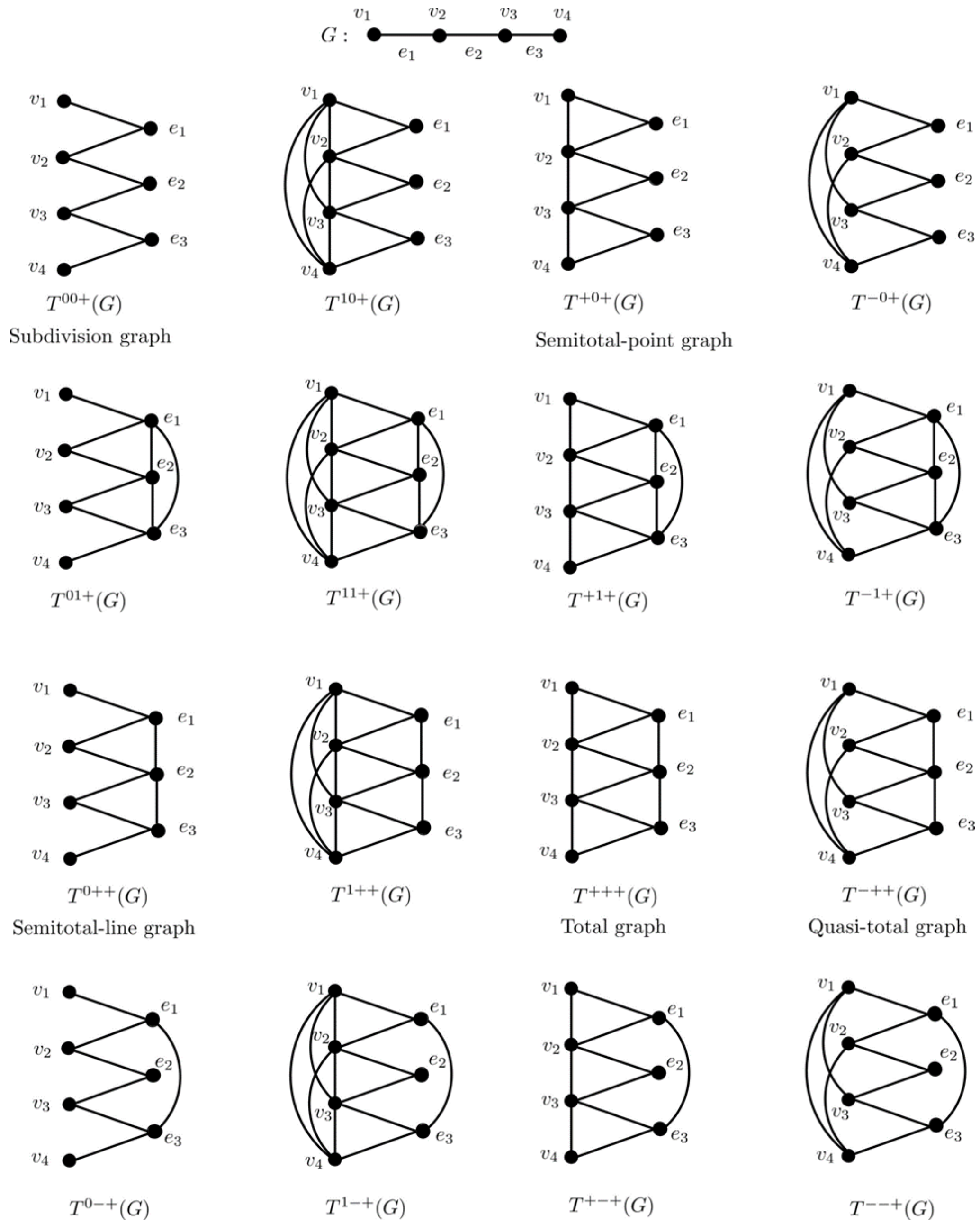
$$LM_3(G) = \sum_{v\in V(G)} d_1(v/G)\cdot d_2(v/G). \qquad (1.3)$$

In[2], Wu Bayoindureng *et al.* introduced the total transformation graphs and obtained the basic properties of total transformation graphs. In[8], Deng *et al.* introduced few more graph operations depending on $x, y, z \in \{0,1,+,-\}$. These graph operations depending on $x, y, z \in \{0,1,+,-\}$ induce functions $T^{xyz}: \mathcal{G} \to \mathcal{G}$. For a graph $G=(V,E)$, let G^0 be the graph with $V(G^0)=V(G)$ and with no edges, G^1 the complete graph with $V(G^1)=V(G)$, $G^+=G$, and $G^-=\overline{G}$. Let $\mathcal{G}$ denotes the set of simple graphs. They referred these resulting graphs as xyz-transformations of G, denoted by $T^{xyz}(G)=G^{xyz}$ and obtained the Laplacian characteristic polynomials and some other Laplacian parameters of xyz-transformations of an r-regular graph G. Further, Basavanagoud[3] established the basic properties of these xyz-transformation graphs by calling them xyz*-point-line transformation graphs*.

Definition 1.[8] *Given a graph* G *with vertex set* $V(G)$ *and edge set* $E(G)$ *and three variables* $x, y, z \in \{0,1,+,-\}$, *the* xyz*-point-line transformation graph* $T^{xyz}(G)$ *of* G *is the graph with vertex set* $V(T^{xyz}(G))=V(G)\cup E(G)$ *and the edge set* $E(T^{xyz}(G))=E((G)^x)\cup E((L(G))^y)\cup E(W)$ *where* $W=S(G)$ *if* $z=+$, $W=\overline{S}(G)$ *if* $z=-$, W *is the graph with* $V(W)=V(G)\cup E(G)$ *and with no edges if* $z=0$ *and* W *is the complete bipartite graph with parts* $V(G)$ *and* $E(G)$ *if* $z=1$.

Since there are 64 distinct 3-permutations of $\{0,1,+,-\}$. Thus obtained 64 kinds of generalized xyz*-point-line transformation graphs*. There are 16 different graphs for each case when $z=0$, $z=1$, $z=+$, $z=-$. In this paper, we consider the xyz*-point-line transformation graphs* $T^{xyz}(G)$ when $z=+$ and then we obtain their leap Zgreb indices. These indices have good correlation with the physico-chemical properties of the chemical compounds for details refer [6].

For instance, the total graph $T(G)$ is a graph with vertex set $V(G)\cup E(G)$ and two vertices of $T(G)$ are adjacent whenever they are adjacent or incident in G. The xyz-point-line transformation graph $T^{--+}(G)$ is a graph with vertex set $V(G)\cup E(G)$ and two vertices of $T^{--+}(G)$ are adjacent whenever they are nonadjacent or incident in G. The self-explanatory examples of the path P_4 and its xyz-*point-line transformation graphs* $T^{xy+}(P_4)$ are depicted in the Figure 1.



$T^{00+}(G)$ Subdivision graph; $T^{10+}(G)$; $T^{+0+}(G)$ Semitotal-point graph; $T^{-0+}(G)$

$T^{01+}(G)$; $T^{11+}(G)$; $T^{+1+}(G)$; $T^{-1+}(G)$

$T^{0++}(G)$ Semitotal-line graph; $T^{1++}(G)$; $T^{+++}(G)$ Total graph; $T^{-++}(G)$ Quasi-total graph

$T^{0-+}(G)$; $T^{1-+}(G)$; $T^{+-+}(G)$; $T^{--+}(G)$

Figure 1.

The following theorems are useful for proving our main results.

Theorem 1.1.[21] *For any graph* G *of order* n *and size* m, $M_1(\overline{G}) = M_1(G) + n(n-1)^2 - 4m(n-1)$. **Theorem 1.2.**[13] *If* G *is any graph of order* n *and size* m, *then* $M_1(G) + \overline{M_1}(G) = 2m(n-1)$.

Theorem 1.3.[1] *If* G *is a simple graph, then* $\overline{M_1}(G) = \overline{M_1}(\overline{G})$.

Theorem 1.4.[9] *If* G *is a graph of order* n *and size* m, *then*

$$\begin{aligned}
M_2(\overline{G}) &= \frac{1}{2}n(n-1)^3 - 3m(n-1)^2 + 2m^2 + \left(\frac{2n-3}{2}\right)M_1(G) - M_2(G),\\
\overline{M_2}(G) &= 2m^2 - \frac{1}{2}M_1(G) - M_2(G),\\
\overline{M_2}(\overline{G}) &= m(n-1)^2 - (n-1)M_1(G) + M_2(G).
\end{aligned}$$

Lemma 1.5.[20] *If* G *is a connected graph of order* n, *then* $d_2(v/G) \le \left(\sum_{u\in N_1(v/G)} d_1(u/G)\right) - d_1(v/G)$. *Equality holds if and only if* G *is* $\{C_3, C_4\}$ *free graph.*

Lemma 1.6.[20] *If* G *is a connected graph of order* n, *then for any vertex* $v \in V(G)$, $d_2(v/G) \le n-1-d_1(v/G) - e(v/G)$.

Observation 1.7.[17] *If* G *is a connected graph of order* n, *then for any vertex* $v \in V(G)$, $d_2(v/G) \le d_1(v/\overline{G}) = n-1-d_1(v/G)$. *Equality holds if and only if* G *has diameter at most two.*

Corollary 1.8.[17] *If* G *is a connected graph of order* n *and size* m *with radius* r, *then*

$$\begin{aligned}
LM_1(G) - M_1(G) &\le (n+1-r)[n^2 - (r-1)n - 4m],\\
LM_2(G) - M_2(G) &\le \frac{m}{n}(n+1-r)[n^2 - (r-1)n - 4m],\\
LM_3(G) + M_1(G) &\le 2m(n+1-r).
\end{aligned}$$

These bounds are sharp and the cycles C_n, $n = 4, 5, 6,$ are attending them.

Proposition 1.9.[17] *Let* G *be a graph of order* n *and size* m. *Then*

$$\begin{aligned} LM_1(G)+LM_1(\overline{G}) &\leq M_1(G)+M_1(\overline{G}),\\ LM_2(G)+LM_2(\overline{G}) &\leq \overline{M_2}(G)+\overline{M_2}(\overline{G}),\\ LM_3(G)+LM_3(\overline{G}) &\leq \overline{M_1}(G)+\overline{M_1}(\overline{G}). \end{aligned}$$

2. LEAP ZAGREB INDICES OF $T^{xy+}(G)$

Theorem 2.1.[5] *Let G be a graph of order n, size m. Let v be the point-vertex of $T^{xy+}(G)$ and e be the line-vertex of $T^{xy+}(G)$ corresponding to a vertex v of G and to an edge e of G, respectively. Then*

$$d_{T^{xy+}(G)}(v)=\begin{cases} d_G(v) & if\ x=0, y\in\{0,1,+,-\}\\ n-1+d_G(v) & if\ x=1, y\in\{0,1,+,-\}\\ 2d_G(v) & if\ x=+, y\in\{0,1,+,-\}\\ n-1 & if\ x=-, y\in\{0,1,+,-\}, \end{cases}$$

$$d_{T^{xy+}(G)}(e)=\begin{cases} 2 & if\ x=0, y\in\{0,1,+,-\}\\ m+1 & if\ x=1, y\in\{0,1,+,-\}\\ 2+d_G(e) & if\ x=+, y\in\{0,1,+,-\}\\ m+1-d_G(e) & if\ x=-, y\in\{0,1,+,-\}. \end{cases}$$

In this paper, we denote $d_1(x/T^{xy+}(G))$ instead of $d_{T^{xy+}(G)}(x)$, where x is either a vertex or an edge of G. We use the following notations while proving our results:

(i) $D_1(e/G)$: The number of vertices of $N_G(u)\cup N_G(v)\ \backslash\{u,v\}$ which are adjacent in G, where $e=uv\in E(G)$.

(ii) $D_2(e/G)=|N_G(u)\cap N_G(v)|$, where $e=uv\in E(G)$.

(iii) $\overline{D_2}(e/G)=|\overline{N_G}(u)\cap\overline{N_G}(v)|$, where $e=uv\in E(G)$ and $\overline{N_G}(v)=\{u\in V(G): u\notin N_G(v)\}$.

(iv) $D_3(v/G)$: The number of vertices of $N_G(v)$ which are adjacent in G, where $v\in V(G)$.

(v) $\overline{D_4}(v/G)=|\bigcup_{e\sim v}\overline{N_G}(u)|$, where $v\in V(G)$ and $e=uv\in E(G)$.

Observation 2.2. *If G is a graph of order n and size m, then for any vertex $v\in V(G)$, $d_2(v/G)\leq n-2$.*

Observation 2.3. *If* G *is a graph of order* n *and size* m*, then* $\sum\limits_{v\in V(G)} d_2(v/G) \le (n-1)(n-2),$ *equality holds if and only if* $G \cong K_{1,n-1.}$

Theorem 2.4. *If* G *is a graph of order* n *and size* m*, then* $0 \le LM_1(G) \le (n-1)(n-2)^2.$

$$(2.1)$$

Upper bound attains if and only if $G \cong K_{1,n-1}$, and lower bound attains if and only if G is a complete graph.

Proof. $LM_1(G) \ge 0$ is trivial. From Observation 2.3, we have

$$\sum_{v\in V(G)} (d_2(v/G))^2 \le (n-1)(n-2)^2. \tag{2.2}$$

Substituting Eq. (2.2) in Eq. (1.1), we get $LM_1(G) \le (n-1)(n-2)^2.$

Thus, $0 \le LM_1(G) \le (n-1)(n-2)^2.$

It is easy to see that, if $G \cong K_{1,n-1}$, then $LM_1(G) = (n-1)(n-2)^2.$

The following proposition gives the 2-distance degree of vertices in the graphs $T^{xy+}(G)$.

Proposition 2.5. *If* G *is a connected* (n,m)*-graph, then*

(i) $d_2(v/T^{10+}(G)) = \begin{cases} m - d_1(v/G) & \text{if } v \in V(G), \\ n-2+d_1(e/G) & \text{if } v = e \in E(G). \end{cases}$

(ii) $d_2(v/T^{11+}(G)) = \begin{cases} m - d_1(v/G) & \text{if } v \in V(G), \\ n-2 & \text{if } v = e \in E(G). \end{cases}$

(iii) $d_2(v/T^{-1+}(G)) = \begin{cases} m & \text{if } v \in V(G), \\ n-2 & \text{if } v = e \in E(G). \end{cases}$

(iv) $d_2(v/T^{1-+}(G)) = \begin{cases} m - d_1(v/G) & \text{if } v \in V(G), \\ n-2+d_1(e/G) & \text{if } v = e \in E(G). \end{cases}$

(v) $d_2(v/T^{+1+}(G)) = \begin{cases} d_2(v/G) - d_1(v/G) + m & \text{if } v \in V(G), \\ n-2 & \text{if } v = e \in E(G). \end{cases}$

(vi) $d_2(v/T^{01+}(G)) = \begin{cases} m & \text{if } v \in V(G), \\ n-2 & \text{if } v = e \in E(G). \end{cases}$

(vii) $d_2(v/T^{-0+}(G)) = \begin{cases} m - D_3(v/G) & \text{if } v \in V(G), \\ 2(n-2) - \overline{D_2}(e/G) & \text{if } v = e \in E(G). \end{cases}$

$$(viii)\ d_2(v/T^{1++}(G))=\begin{cases} m-d_1(v/G) & if\ v\in V(G),\\ n-2+\sum\limits_{z\in(N_G(u)\cup N_G(w))}(d_1(z/G)-1)-[D_1(e/G)+D_2(e/G)] & if\ v=e\in E(G).\end{cases}$$

$$(ix)\ d_2(v/T^{-++}(G))=\begin{cases} m & if\ v\in V(G),\\ n-2+\sum\limits_{z\in(N_G(u)\cup N_G(w))}(d_1(z/G)-1)-[D_1(e/G)+D_2(e/G)] & if\ v=e\in E(G).\end{cases}$$

$$(\mathrm{x})\ d_2(v/T^{0-+}(G))=\begin{cases} d_1(v/G)+\overline{D_4}(v/G) & if\ v\in V(G),\\ n-2+d_1(e/G) & if\ v=e\in E(G).\end{cases}$$

$$(\mathrm{xi})\ d_2(v/T^{+-+}(G))=\begin{cases} 2d_2(v/G)+\overline{D_4}(v/G) & if\ v\in V(G),\\ n-2+d_1(e/G) & if\ v=e\in E(G).\end{cases}$$

$$(\mathrm{xii})\ d_2(v/T^{--+}(G))=\begin{cases} m & if\ v\in V(G),\\ n-2+d_1(e/G) & if\ v=e\in E(G).\end{cases}$$

$$(\mathrm{xiii})\ d_2(v/T^{00+}(G))=\begin{cases} d_1(v/G) & if\ v\in V(G),\\ d_1(e/G) & if\ v=e\in E(G).\end{cases}$$

$$(\mathrm{xiv})\ d_2(v/T^{+0+}(G))=\begin{cases} d_2(v/G)+\left[\sum\limits_{u\in N_G(v)}d_1(u/G)\right]-d_1(v/G)-D_3(v/G) & if\ v\in V(G),\\ 2d_1(e/G)-D_2(e/G) & if\ v=e\in E(G).\end{cases}$$

$$(xv)\ d_2(v/T^{0++}(G))=\begin{cases} \left[\sum\limits_{u\in N_G(v)}d_1(u/G)\right]-D_3(v/G) & if\ v\in V(G),\\ \left[\sum\limits_{z\in(N_G(u)\cup N_G(w))\backslash\{u,w\}}d_1(z/G)\right]-[D_1(e/G)+D_2(e/G)] & if\ v=e\in E(G).\end{cases}$$

$$(xvi)\ d_2(v/T^{+++}(G))=\begin{cases} d_2(v/G)+\left[\sum\limits_{u\in N_G(v)}d_1(u/G)\right]-d_1(v/G)-D_3(v/G) & if\ v\in V(G),\\ \left[\sum\limits_{z\in(N_G(u)\cup N_G(w))\backslash\{u,w\}}d_1(z/G)\right]-[D_1(e/G)+D_2(e/G)] & if\ v=e\in E(G).\end{cases}$$

In literature, the graphs $T^{00+}(G), T^{+0+}(G), T^{0++}(G), T^{+++}(G)$ and $T^{-++}(G)$ are known as Subdivision graph[12] $S(G)$, Semitotal-point graph[18] $T_2(G)$, Semitotal-line graph (or Middle graph)[11] $T_1(G)$ Total graph[12] $T(G)$ and Quasi total graph[19] $P(G)$, respectively. We obtain the leap Zagreb indices of the xyz *-point-line transformation graphs* $T^{xy+}(G)$ in the following theorems. The leap Zagreb indices of the xyz *-point-line transformation graphs* $T^{xy1}(G)$ can be found in[7]. Let n vertices of the graph G be $v_1, v_2, ..., v_n$, and let $e_1, e_2, ..., e_m$ be the line vertices of G, where $n \geq 2$ and $m \geq 1$.

Theorem 2.6. *If* G *is a connected graph with* n *vertices and* m *edges, then*

$$LM_1(T^{xyz}(G)) \leq (n+m-1)(n+m-2)^2.$$

Equality hold, if and only if $G \cong K_2$ *for* $T^{xyz}(G) = S(G), T_1(G)$.

Theorem 2.7. *If* G *is a connected graph with* n *vertices and* m *edges, then*

$$\begin{aligned} LM_1(T^{xyz}(G)) &\leq M_1(\overline{T^{xyz}(G)}), \\ LM_1(T^{xyz}(G)) &\leq n(n-1)^2 - 2m(n-1) - \overline{M_1}(T^{xyz}(G)), \\ LM_2(T^{xyz}(G)) &\leq \overline{M_2}(\overline{T^{xyz}(G)}), \\ LM_3(T^{xyz}(G)) &\leq \overline{M_1}(\overline{T^{xyz}(G)}) = \overline{M_1}(T^{xyz}(G)). \end{aligned}$$

Equality hold, if and only if

$$G \cong \begin{cases} nK_1 \text{ or } K_2 & \text{when } S(G), \\ nK_1 \text{ or } K_3 \text{ or } K_{1,n} \text{ or } P_n, n \leq 3 & \text{when } T_2(G), \\ nK_1 \text{ or } K_n & \text{when } T_1(G), \\ nK_1 \text{ or } K_n \text{ or } K_{1,n} \text{ or } W_{1,4} & \text{when } T(G). \end{cases}$$

The following theorem is an illustration to above inequalities for $T^{xyz}(G) = S(G)$ as an example. These inequalities can also be obtained for other *generalized* xyz *-point-line transformation graphs* in the similar manner.

Theorem 2.8. *If* G *is a graph of order* n *and size* m, *then*

$$LM_1[S(G)] \leq (n+m-1)[(n+m)^2 - n - 9m] + M_1(G) + 4m, \tag{2.3}$$

$$LM_2[S(G)] \leq 2m(n+m-1)(n+m-3) - (n+m-3)M_1(G), \tag{2.4}$$

$$LM_3[S(G)] \leq 4m(n+m-2) - M_1(G). \tag{2.5}$$

Equality holds if and only if G is either nK_1 or K_2.

Proof. We prove only the inequality (2.3). The proofs of the inequalities (2.4) and (2.5) are analogous. From Observation 1.7, Proposition 2.5 (xiii) and the fact that

$$d_1(v/S(G)) = \begin{cases} d_1(v/G) & \text{if } v \in V(G), \\ 2 & \text{if } v \in E(G), \end{cases}$$ we have

$$\begin{aligned} LM_1[S(G)] &\leq \sum_{v\in V(S(G))}[n+m-1-d_1(v/S(G))]^2 \\ &= \sum_{v\in V(G)}[n+m-1-d_1(v/G)]^2+\sum_{v\in E(G)}[n+m-1-2]^2 \\ &= n(n+m-1)^2-4m(n+m-1)+M_1(G)+m(n+m-3)^2 \\ &= (n+m-1)[(n+m)^2-n-9m]+M_1(G)+4m. \end{aligned}$$

Suppose G has diameter at most two. Then we have the following.
If $diam(S(G))=2$, then by Observation 1.7, $d_2(v/S(G))=n+m-1-d_1(v/S(G))$, for every $v\in V(S(G))$. Hence,

$$\begin{aligned} LM_1[S(G)] &= \sum_{v\in V(S(G))} d_2(v/S(G))^2 = \sum_{v\in V(S(G))} d_1(v/\overline{S(G)})^2 = \sum_{v\in V(S(G))}[n+m-1-d_1(v/S(G))]^2 \\ &= \sum_{v\in V(G)}[n+m-1-d_1(v/G)]^2+\sum_{v\in E(G)}[n+m-1-2]^2 \\ &= n(n+m-1)^2-4m(n+m-1)+M_1(G)+m(n+m-3)^2 \\ &= (n+m-1)[(n+m)^2-n-9m]+M_1(G)+4m. \end{aligned}$$

Suppose on contrary, that $diam(S(G))\geq 3$. Then there is at least one vertex v such that $e(v/S(G))\geq diam(S(G))\geq 3.$ Thus $d_2(v/S(G))\leq d_1(v/S(G))$, for every vertex v with $e(v/S(G))\geq 3.$ Therefore,

$$LM_1[S(G)]<\sum_{v\in V(S(G))}[n+m-1-d_1(v/S(G))]^2=(n+m-1)[(n+m)^2-n-9m]+M_1(G)+4m.$$

Theorem 2.9.1 *If G is a graph of order n and size m, then*
$LM_1[S(G)]=M_1(G)+EM_1(G).$

Proof. We know that, the subdivision graph $S(G)$ has $n+m$ vertices and $2m$ edges. Therefore, by Eq. (1.1) and Proposition 2.5 (xiii), we have

$$\begin{aligned} LM_1[S(G)] &= \sum_{v\in V(S(G))}[d_2(v/S(G))]^2 \\ &= \sum_{v\in V(G)}[d_2(v/S(G))]^2+\sum_{e\in E(G)} d_2(e/S(G)) \\ &= \sum_{v\in V(G)}[d_1(v/G)]^2+\sum_{e\in E(G)} d_1(e/G) \\ &= M_1(G)+EM_1(G). \end{aligned}$$

Theorem 2.10. *If G is a graph of order n and size m, then*
$LM_2[S(G)]=F(G)+2(M_2(G)-M_1(G)).$

Proof. We know that, the subdivision graph $S(G)$ has $n+m$ vertices and $2m$ edges. Therefore, by using Eq. (1.2) and Proposition 2.5 (xiii), we have

$$\begin{aligned}
LM_2[S(G)] &= \sum_{uv\in E(S(G))} d_2(u/S(G))\cdot d_2(v/S(G)) \\
&= \sum_{uv\in E(S(G))} d_1(u/G)\cdot d_1(e/G), \quad \text{where } v=e\in E(G) \\
&= \sum_{uw\in E(G)} d_1(e/G)[d_1(u/G)+d_1(w/G)] \\
&= \sum_{uw\in E(G)} [d_1(u/G)+d_1(w/G)-2][d_1(u/G)+d_1(w/G)] \\
&= \sum_{uw\in E(G)} [d_1(u/G)+d_1(w/G)]^2 - 2\sum_{uw\in E(G)} [d_1(u/G)+d_1(w/G)] \\
&= \sum_{uw\in E(G)} [d_1(u/G)^2+d_1(w/G)^2] + 2\sum_{uw\in E(G)} d_1(u/G)d_1(w/G) - 2M_1(G) \\
&= F(G) + 2(M_2(G)-M_1(G)).
\end{aligned}$$

Theorem 2.11. *If G is a graph of order n and size m, then $LM_3[S(G)] = 3M_1(G)-4m.$*

Proof. We know that, the subdivision graph $S(G)$ has $n+m$ vertices and $2m$ edges. For a vertex $v\in S(G)$, $d_1(v/S(G)) = \begin{cases} d_1(v/G) & \text{if } v\in V(G), \\ 2 & \text{if } v=e\in E(G). \end{cases}$

Therefore, by using Eq. (1.3) and Proposition 2.5 (xiii), we have

$$\begin{aligned}
LM_3[S(G)] &= \sum_{v\in V(S(G))} d_1(v/S(G))\cdot d_2(v/S(G)) \\
&= \sum_{v\in V(G)} d_1(v/S(G))\cdot d_2(v/S(G)) + \sum_{e\in E(G)} d_1(e/S(G))\cdot d_2(e/S(G)) \\
&= \sum_{v\in V(G)} d_1(v/G)\cdot d_1(v/G) + \sum_{e\in E(G)} 2d_1(e/G) \\
&= 3M_1(G)-4m.
\end{aligned}$$

Theorem 2.12. *If G is a graph of order n and size m, then*

$$\begin{aligned}
LM_1[T_2(G)] = {} & LM_1(G) + \sum_{v\in V(G)} \left(\sum_{u\in N_G(v)} d_1(u/G) \right)^2 + 2\sum_{v\in V(G)} d_2(v/G) \left(\sum_{u\in N_G(v)} d_1(u/G) \right) \\
& - 2\sum_{v\in V(G)} \left(d_2(v/G) \sum_{u\in N_G(v)} d_1(u/G) \right) (d_1(v/G)+D_3(v/G)) + M_1(G) + \sum_{v\in V(G)} D_3(v/G)^2 \\
& + 2\sum_{v\in V(G)} d_1(v/G)D_3(v/G) + 4EM_1(G) + \sum_{e\in E(G)} D_2(e/G)^2 - 4\sum_{e\in E(G)} d_1(e/G)D_2(e/G).
\end{aligned}$$

Proof. We know that, the semitotal-point graph $T_2(G)$ has $n+m$ vertices and $3m$ edges. Therefore, by using Eq. (1.1) and Proposition 2.5 (xiv), we have

$$\begin{aligned}
LM_1[T_2(G)] &= \sum_{v\in V(G)} d_2(v/T_2(G))^2 \\
&= \sum_{v\in V(G)} \left[d_2(v/G) + \left(\sum_{u\in N_G(v)} d_1(u/G) \right) - d_1(v/G) - D_3(v/G) \right]^2 \\
&= LM_1(G) + \sum_{v\in V(G)} \left[\sum_{u\in N_G(v)} d_1(u/G) \right]^2 + 2\sum_{v\in V(G)} d_2(v/G) \left(\sum_{u\in N_G(v)} d_1(u/G) \right) \\
&\quad - 2\sum_{v\in V(G)} \left[d_2(v/G) \sum_{u\in N_G(v)} d_1(u/G) \right] [d_1(v/G) + D_3(v/G)] + M_1(G) + \sum_{v\in V(G)} D_3(v/G)^2 \\
&\quad + 2\sum_{v\in V(G)} d_1(v/G) D_3(v/G) + 4EM_1(G) + \sum_{e\in E(G)} D_2(e/G)^2 - 4\sum_{e\in E(G)} d_1(e/G) D_2(e/G).
\end{aligned}$$

Theorem 2.13. *If G is a graph of order n and size m, then*

$$\begin{aligned}
LM_2[T_2(G)] &= \sum_{uv\in E(T_2(G)), v\in E(G)} \left[d_2(u/G) + \left(\sum_{w\in N_G(u)} d_1(w/G) \right) - d_1(u/G) - D_3(u/G) \right] \\
&\quad [2d_1(e/G) - D_2(e/G)],
\end{aligned}$$

where $v = e \in E(G)$.

Proof. We know that, the semitotal-point graph $T_2(G)$ has $n+m$ vertices and $3m$ edges and $uv \in E(T_2(G))$ means u ia a vertex and $v = e$ is an edge of the graph G. Therefore, by using Eq. (1.2) and Proposition 2.5 (xiv), we have

$$\begin{aligned}
LM_2[T_2(G)] &= \sum_{uv\in E(T_2(G))} d_2(u/T_2(G)) d_2(v/T_2(G)) \\
&= \sum_{uv\in E(T_2(G)), v\in E(G)} \left[d_2(u/G) \left(\sum_{w\in N_G(u)} d_1(w/G) \right) - d_1(u/G) - D_3(u/G) \right] \\
&\quad [2d_1(e/G) - D_2(e/G)].
\end{aligned}$$

Theorem 2.14. *If G is a graph of order n and size m, then*

$$\begin{aligned}
LM_3[T_2(G)] &= 2LM_3(G) + 2M_1(G) - 8m + 2\sum_{v\in V(G)} d_1(v/G) \left[\left(\sum_{u\in N_G(v)} d_1(u/G) \right) - D_3(v/G) \right] \\
&\quad - 2\sum_{e\in E(G)} D_2(e/G).
\end{aligned}$$

Proof. We know that, the semitotal-point graph $T_2(G)$ has $n+m$ vertices, $3m$ edges. For a vertex $v \in T_2(G)$, $d_1(v/T_2(G)) = \begin{cases} 2d_1(v/G) & if \ v \in V(G), \\ 2 & if \ v = e \in E(G). \end{cases}$

Therefore, by using Eq. (1.3) and Proposition 2.5 (xiv), we have

$$\begin{aligned} LM_3[T_2(G)] &= \sum_{v\in V(T_2(G))} d_1(v/T_2(G)) \cdot d_2(v/T_2(G)) \\ &= \sum_{v\in V(G)} 2d_1(v/G)\left[d_2(v/G) + \left(\sum_{u\in N_G(v)} d_1(u/G) \right) - d_1(v/G) - D_3(v/G) \right] \\ &\quad + \sum_{e\in E(G)} 2[2d_1(e/G) - D_2(e/G)] \\ &= 2LM_3(G) + 2M_1(G) - 8m + 2\sum_{v\in V(G)} d_1(v/G)\left[\left(\sum_{u\in N_G(v)} d_1(u/G) \right) - D_3(v/G) \right] \\ &\quad - 2\sum_{e\in E(G)} D_2(e/G). \end{aligned}$$

Theorem 2.15. *If G is a graph of order n and size m, then*

$$\begin{aligned} LM_1[T_1(G)] &= \sum_{v\in V(G)} \left[\left(\sum_{u\in N_G(v)} d_1(u/G) \right) - D_3(v/G) \right]^2 \\ &\quad + \sum_{e\in E(G)} \left[\left(\sum_{z\in (N_G(u)\cup N_G(v))\backslash\{u,v\}} d_1(z/G) \right) - (D_1(e/G) + D_2(e/G)) \right]^2 . \end{aligned}$$

Proof. The proof is immediate by using Eq. (1.1) and Proposition 2.5 (xv).

Theorem 2.16. *Let G be a graph of order n and size m. Let $u_1 = uv, v_1 = vw \in E(G)$ and $e = xy \in E(G)$. Then*

$$\begin{aligned} LM_2[T_1(G)] &= \sum_{uv\in E(T_1(G)), v=e\in E(G)} \left[\left(\sum_{w\in N_G(u)} d_1(w/G) \right) - D_3(u/G) \right] \\ &\qquad \left[\left(\sum_{z_1\in (N(x)\cup N(y))\backslash\{x,y\}} d_1(z_1/G) \right) - (D_1(e/G) + D_2(e/G)) \right] \\ &\quad + \sum_{u_1v_1\in E(T_1(G)), u_1, v_1\in E(G)} \left[\left(\sum_{z_2\in (N(u)\cup N(v))\backslash\{u,v\}} d_1(z_2/G) \right) - (D_1(u_1/G) + D_2(u_1/G)) \right] \\ &\qquad \left[\left(\sum_{z_3\in (N(u)\cup N(w))\backslash\{u,v\}} d_1(z_3/G) \right) - (D_1(u_2/G) + D_2(u_2/G)) \right]. \end{aligned}$$

Proof. The proof is immediate by using Eq. (1.2) and Proposition 2.5 (xv).

Theorem 2.17. *If* G *is a graph of order* n, *size* m *and* $e = uv \in E(G)$, *then*

$$\begin{aligned} LM_3[T_1(G)] &= \sum_{v\in V(G)} d_1(v/G)\left[\left(\sum_{u\in N_G(v)} d_1(u/G)\right) - D_3(v/G)\right] \\ &\quad + \sum_{e\in E(G)} (2+d_1(e/G))\left[\left(\sum_{z\in(N(u)\cup N(v))\setminus\{u,v\}} d_1(z/G)\right) - (D_1(e/G)+D_2(e/G))\right]. \end{aligned}$$

Proof. The proof is immediate by using Eq. (1.3), Proposition 2.5 (xv) and the fact that

$$d_1(v/T_1(G)) = \begin{cases} d_1(v/G) & \text{if } v\in V(G), \\ 2+d_1(e/G) & \text{if } v = e\in E(G). \end{cases}$$

Theorem 2.18. *If* G *is a graph of order* n *and size* m, *then*

$$\begin{aligned} LM_1[T(G)] &= LM_1(G) + \sum_{v\in V(G)}\left(\sum_{u\in N_G(v)} d_1(u/G)\right)^2 + 2\sum_{v\in V(G)} d_2(v/G)\left(\sum_{u\in N_G(v)} d_1(u/G)\right) \\ &\quad - 2LM_3(G) - \sum_{v\in V(G)} d_2(v/G)D_3(v/G) - \sum_{v\in V(G)}\left(\sum_{u\in N_G(v)} d_1(u/G)\right)[d_1(v/G)+D_3(v/G)] + M_1(G) \\ &\quad + \sum_{v\in V(G)} D_3(v/G)^2 + 2\sum_{v\in V(G)} d_1(v/G)D_3(v/G) + \sum_{e\in E(G)}\left(\sum_{z\in(N_G(u)\cup N_G(v))\setminus\{u,v\}} d_1(z/G)\right)^2 \end{aligned}$$

$$\begin{aligned} &-2\sum_{e\in E(G)}\left[\left(\sum_{z\in(N_G(u)\cup N_G(v))\setminus\{u,v\}} d_1(z/G)\right)(D_1(e/G)+D_2(e/G))\right] + \sum_{e\in E(G)} D_1(e/G)^2 \\ &+ \sum_{e\in E(G)} D_2(e/G)^2 + \sum_{e\in E(G)} D_1(e/G)D_2(e/G). \end{aligned}$$

Proof. The proof is immediate by using Eq. (1.1) and Proposition 2.5 (xvi).

Theorem 2.19. *Let* G *be a graph of order* n *and size* m. *Let* $u_1 = uv, v_1 = vw \in E(G)$ *and* $e = xy \in E(G)$. *Then*

$$\begin{aligned} LM_2[T(G)] &= \sum_{uv\in E(T_1(G)), v=e\in E(G)}\left[\left(\sum_{w\in N_G(u)} d_1(w/G)\right) - D_3(u/G)\right] \\ &\qquad \left[\left(\sum_{z\in(N(x)\cup N(y)\setminus\{x,y\}} d_1(z/G)\right) - (D_1(e/G)+D_2(e/G))\right] \\ &\quad + \sum_{u_1v_1\in E(T_1(G)), u_1,v_1\in E(G)}\left[\left(\sum_{z\in(N(u)\cup N(v)\setminus\{u,v\}} d_1(z/G)\right) - (D_1(u_1/G)+D_2(u_1/G))\right] \\ &\qquad \left[\left(\sum_{z\in(N(v)\cup N(w)\setminus\{v,w\}} d_1(z/G)\right) - (D_1(u_2/G)+D_2(u_2/G))\right]. \end{aligned}$$

Proof. The proof is immediate by using Eq. (1.2) and Proposition 2.5 (xvi).

Theorem 2.20. *If* G *is a graph of order* n, *size* m *and* $e = uv \in E(G)$, *then*

$$\begin{aligned} LM_3[T(G)] &= \sum_{v\in V(G)} d_1(v/G)\left[\left(\sum_{u\in N_G(v)} d_1(u/G)\right) - D_3(v/G)\right] \\ &\quad + \sum_{e\in E(G)} (2+d_1(e/G))\left[\left(\sum_{z\in(N_G(u)\cup N_G(v))\setminus\{u,v\}} d_1(z/G)\right) - (D_1(e/G)+D_2(e/G))\right]. \end{aligned}$$

Proof. The proof is immediate by using Eq. (1.3), Proposition 2.5 (xvi) and the fact that

$$d_1(v/T(G)) = \begin{cases} 2d_1(v/G) & if\ v\in V(G), \\ 2+d_1(e/G) & if\ v = e\in E(G). \end{cases}$$

Theorem 2. *For the graph* $T^{10+}(G)$ *of a graph* G, *the leap Zagreb indices are given by*

$$\begin{aligned} LM_1(T^{10+}(G)) &= m(mn+n^2-8n+8)+(2n-3)M_1(G)+EM_1(G); \\ LM_2(T^{10+}(G)) &= \frac{1}{2}m^2(n^2-n-8)+\frac{1}{2}(4m-2n+7)M_1(G)-2M_2(G)-F(G); \\ LM_3(T^{10+}(G)) &= 2m(m-3)+mn(n-1)+M_1(G). \end{aligned}$$

Proof. From Eq. (1.1), we have

$$\begin{aligned} LM_1(T^{10+}(G)) &= \sum_{v\in V(T^{10+}(G))} d_2(v/T^{10+}(G))^2 \\ &= \sum_{v\in V(G)} d_2(v/T^{10+}(G))^2 + \sum_{e\in E(G)} d_2(e/T^{10+}(G))^2. \end{aligned}$$

By using Proposition 2.5(i), we obtain

$$\begin{aligned} &= \sum_{v\in V(G)} (m-d_1(v/G))^2 + \sum_{e\in E(G)} (n-2+d_1(e/G))^2 \\ &= m(mn+n^2-8n+8)+(2n-3)M_1(G)+EM_1(G). \end{aligned}$$

Next, from Eq. (1.2), we have

$$\begin{aligned} LM_2(T^{10+}(G)) &= \sum_{uv\in E(T^{10+}(G))} d_2(u/T^{10+}(G))\cdot d_2(v/T^{10+}(G)) \\ &= \sum_{uv\in E(T^{10+}(G)),u,v\in V(G)} d_2(u/T^{10+}(G))\cdot d_2(v/T^{10+}(G)) \\ &\quad + \sum_{uv\in E(T^{10+}(G)),u\in V(G),v\in E(G)} d_2(u/T^{10+}(G))\cdot d_2(v/T^{10+}(G)) \\ &= \frac{1}{2}\sum_{u,v\in V(G)} d_2(u/T^{10+}(G))\cdot d_2(v/T^{10+}(G)) + \sum_{uv\in E(S(G))} d_2(u/T^{10+}(G))\cdot d_2(v/T^{10+}(G)). \end{aligned}$$

By using Proposition2.5(i), we obtain

$$\begin{aligned} &= \frac{1}{2}\sum_{u,v\in V(G)} (m-d_1(u/G))(m-d_1(v/G)) + \sum_{uv\in E(S(G))} (m-d_1(u/G))(n-2+d_1(v/G)) \\ &= \frac{1}{2}m^2(n^2-n-8)+\frac{1}{2}(4m-2n+7)M_1(G)-2M_2(G)-F(G). \end{aligned}$$

Finally, from Eq. (1.3) and the fact that $d_1(v/T^{10+}(G)) = \begin{cases} n-1+d_1(v/G) & \text{if } v\in V(G), \\ 2 & \text{if } v\in E(G), \end{cases}$ we have

$$\begin{aligned} LM_3(T^{10+}(G)) &= \sum_{v\in V(T^{10+}(G))} d_1(v/T^{10+}(G))\cdot d_2(v/T^{10+}(G)) \\ &= \sum_{v\in V(G)} d_1(v/T^{10+}(G))\cdot d_2(v/T^{10+}(G)) + \sum_{v\in E(G)} d_1(v/T^{10+}(G))\cdot d_2(v/T^{10+}(G)). \\ &\text{By using Proposition 2.5(i), we obtain} \\ &= \sum_{v\in V(G)} (n-1+d_1(v/G))(m-d_1(v/G)) + \sum_{v\in E(G)} 2(n-2+d_1(v/G)) \\ &= 2m(m-3)+mn(n-1)+M_1(G). \end{aligned}$$

Theorem 2.22. *For the graph* $T^{11+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$\begin{aligned} LM_1(T^{11+}(G)) &= (n-4)m^2+m(n-2)^2+M_1(G); \\ LM_2(T^{11+}(G)) &= \frac{1}{2}nm^2(n-1)-\frac{1}{2}(2n-3)M_1(G)+\frac{1}{2}m(m-1)(n-2)^2; \\ LM_3(T^{11+}(G)) &= 2m^2+m(n-1)(n-2)-M_1(G)+m(m+1)(n-2). \end{aligned}$$

Proof. From Eq. (1.1), we have

$$\begin{aligned} LM_1(T^{11+}(G)) &= \sum_{v\in V(T^{11+}(G))} d_2(v/T^{11+}(G))^2 \\ &= \sum_{v\in V(G)} d_2(v/T^{11+}(G))^2 + \sum_{e\in E(G)} d_2(e/T^{11+}(G))^2. \\ &\text{By using Proposition 2.5(ii), we obtain} \\ &= \sum_{v\in V(G)} (m-d_1(v/G))^2 + \sum_{e\in E(G)} (n-2)^2 \\ &= (n-4)m^2+m(n-2)^2+M_1(G). \end{aligned}$$

From Eq. (1.2), we have

$$\begin{aligned} LM_2(T^{11+}(G)) &= \sum_{uv\in E(T^{11+}(G))} d_2(u/T^{11+}(G))\cdot d_2(v/T^{11+}(G)) \\ &= \frac{1}{2}\sum_{u,v\in V(G)} d_2(u/T^{11+}(G))\cdot d_2(v/T^{11+}(G)) + \sum_{uv\in E(S(G))} d_2(u/T^{11+}(G))\cdot d_2(v/T^{11+}(G)) \\ &+\frac{1}{2}\sum_{u,v\in E(G)} d_2(u/T^{11+}(G))\cdot d_2(v/T^{11+}(G)). \\ &\text{By using Proposition 2.5(ii), we obtain} \\ &= \frac{1}{2}\sum_{u,v\in V(G)} (m-d_1(u/G))(m-d_1(v/G)) + \sum_{uv\in E(S(G))} (m-d_1(u/G))(n-2) \\ &+\frac{1}{2}\sum_{u,v\in E(G)} (n-2)^2 \\ &= \frac{1}{2}nm^2(n-1)-\frac{1}{2}(2n-3)M_1(G)+\frac{1}{2}m(m-1)(n-2)^2. \end{aligned}$$

Now, from Eq. (1.3) and the fact that $d_1(v/T^{11+}(G)) = \begin{cases} n-1+d_1(v/G) & if\ v\in V(G), \\ m+1 & if\ v\in E(G), \end{cases}$ we have

$$\begin{aligned} LM_3(T^{11+}(G)) &= \sum_{v\in V(T^{11+}(G))} d_1(v/T^{11+}(G))\cdot d_2(v/T^{11+}(G)) \\ &= \sum_{v\in V(G)} d_1(v/T^{11+}(G))\cdot d_2(v/T^{11+}(G)) + \sum_{v\in E(G)} d_1(v/T^{11+}(G))\cdot d_2(v/T^{11+}(G)). \\ &\text{By using Proposition2.5(ii), we obtain} \\ &= \sum_{v\in V(G)} (n-1+d_1(v/G))(m-d_1(v/G)) + \sum_{v\in E(G)} (m+1)(n-2) \\ &= 2m^2 + m(n-1)(n-2) - M_1(G) + m(m+1)(n-2). \end{aligned}$$

Theorem 2.23. *For the graph* $T^{-1+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$\begin{aligned} LM_1(T^{-1+}(G)) &= nm^2 + m(n-2)^2; \\ LM_2(T^{-1+}(G)) &= \frac{1}{2}m^2(n^2-n-2m) + \frac{1}{2}m(n-2)(mn+2m-n+2); \\ LM_3(T^{-1+}(G)) &= m(n^2-2m+mn-2). \end{aligned}$$

Proof. From Eq. (1.1), we have

$$\begin{aligned} LM_1(T^{-1+}(G)) &= \sum_{v\in V(T^{-1+}(G))} d_2(v/T^{-1+}(G))^2 \\ &= \sum_{v\in V(G)} d_2(v/T^{-1+}(G))^2 + \sum_{e\in E(G)} d_2(e/T^{-1+}(G))^2. \\ &\text{By using Proposition 2.5(iii),we obtain} \\ &= \sum_{v\in V(G)} m^2 + \sum_{e\in E(G)} (n-2)^2 \\ &= nm^2 + m(n-2)^2. \end{aligned}$$

Next, from Eq. (1.2), we have

$$\begin{aligned} LM_2(T^{-1+}(G)) &= \sum_{uv\in E(T^{-1+}(G))} d_2(u/T^{-1+}(G))\cdot d_2(v/T^{-1+}(G)) \\ &= \sum_{uv\notin E(G)} d_2(u/T^{-1+}(G))\cdot d_2(v/T^{-1+}(G)) + \sum_{uv\in E(S(G))} d_2(u/T^{-1+}(G))\cdot d_2(v/T^{-1+}(G)) \\ &+ \sum_{u,v\in E(G)} d_2(u/T^{-1+}(G))\cdot d_2(v/T^{-1+}(G)). \\ &\text{By using Proposition 2.5(iii), we obtain} \\ &= \sum_{uv\notin E(G)} m^2 + \sum_{uv\in E(S(G))} m(n-2) + \sum_{u,v\in E(G)} (n-2)^2 \\ &= \frac{1}{2}m^2(n^2-n-2m) + \frac{1}{2}m(n-2)(mn+2m-n+2). \end{aligned}$$

Now, from Eq. (1.3) and the fact that $d_1(v/T^{-1+}(G)) = \begin{cases} n-1 & if\ v \in V(G), \\ m+1 & if\ v \in E(G), \end{cases}$ we have

$$\begin{aligned} LM_3(T^{-1+}(G)) &= \sum_{v\in V(T^{-1+}(G))} d_1(v/T^{-1+}(G)) \cdot d_2(v/T^{-1+}(G)) \\ &= \sum_{v\in V(G)} d_1(v/T^{-1+}(G)) \cdot d_2(v/T^{-1+}(G)) + \sum_{v\in E(G)} d_1(v/T^{-1+}(G)) \cdot d_2(v/T^{-1+}(G)). \end{aligned}$$

By using Proposition 2.5(iii), we obtain

$$\begin{aligned} &= \sum_{v\in V(G)} (n-1)m + \sum_{v\in E(G)} (m+1)(n-2) \\ &= m(n^2 - 2m + mn - 2). \end{aligned}$$

Theorem 2.24. *For the graph* $T^{1-+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$LM_1(T^{1-+}(G)) = (n-4)m^2 + (2n-3)M_1(G) + EM_1(G) + m(n^2 - 8n + 12);$$

$$LM_2(T^{1-+}(G)) = \frac{1}{2}m^2(n^2-n-8) - \frac{1}{2}(n^2-2n-4m-3)M_1(G) + (n-2)\overline{EM_1}(G) + \overline{EM_2}(G)$$

$$-F(G) - 2M_2(G) + \frac{1}{2}m(m+1)(n-2)^2;$$

$$LM_3(T^{1-+}(G)) = 2m^2 + mn(n-1) + (m-n+2)M_1(G) - 2m(m+2) + m(m+1)(n-2) - EM_1(G).$$

Proof. From Eq. (1.1), we have

$$\begin{aligned} LM_1(T^{1-+}(G)) &= \sum_{v\in V(T^{1-+}(G))} d_2(v/T^{1-+}(G))^2 \\ &= \sum_{v\in V(G)} d_2(v/T^{1-+}(G))^2 + \sum_{e\in E(G)} d_2(e/T^{1-+}(G))^2. \end{aligned}$$

By using Proposition 2.5(iv), we obtain

$$\begin{aligned} &= \sum_{v\in V(G)} (m - d_1(v/G))^2 + \sum_{e\in E(G)} (n-2+d_1(e/G))^2 \\ &= (n-4)m^2 + (2n-3)M_1(G) + EM_1(G) + m(n^2 - 8n + 12). \end{aligned}$$

Next, from Eq. (1.2), we have

$$\begin{aligned} LM_2(T^{1-+}(G)) &= \sum_{uv\in E(T^{1-+}(G))} d_2(u/T^{1-+}(G)) \cdot d_2(v/T^{1-+}(G)) \\ &= \sum_{uv\in E(G)} d_2(u/T^{1-+}(G)) \cdot d_2(v/T^{1-+}(G)) + \sum_{uv\notin E(G)} d_2(u/T^{1-+}(G)) \cdot d_2(v/T^{1-+}(G)) \\ &+ \sum_{uv\in E(S(G))} d_2(u/T^{1-+}(G)) \cdot d_2(v/T^{1-+}(G)) \\ &+ \sum_{u,v\in E(G),\, u\nsim v} d_2(u/T^{1-+}(G)) \cdot d_2(v/T^{1-+}(G)). \end{aligned}$$

By using Proposition 2.5 (iv), we obtain

$$= \sum_{uv\in E(G)} (m-d_1(u/G))(m-d_1(v/G)) + \sum_{uv\notin E(G)} (m-d_1(u/G))(m-d_1(v/G))$$

$$+ \sum_{uv\in E(S(G))} (m-d_1(u/G))(n-2+d_1(v/G))$$

$$+ \sum_{u,v\in E(G),\, u\nsim v} (n-2+d_1(u/G))(n-2+d_1(v/G))$$

$$= \frac{1}{2}m^2(n^2-n-8) - \frac{1}{2}(n^2-2n-4m-3)M_1(G) + (n-2)\overline{EM_1}(G) + \overline{EM_2}(G)$$

$$-F(G) - 2M_2(G) + \frac{1}{2}m(m+1)(n-2)^2.$$

Now, from Eq. (1.3) and the fact that

$$d_1(v/T^{1-+}(G)) = \begin{cases} n-1+d_1(v/G) & if\ v\in V(G), \\ m+1-d_1(e/G) & if\ v=e\in E(G), \end{cases}$$ we have

$$LM_3(T^{1-+}(G)) = \sum_{v\in V(T^{1-+}(G))} d_1(v/T^{1-+}(G))\cdot d_2(v/T^{1-+}(G))$$

$$= \sum_{v\in V(G)} d_1(v/T^{1-+}(G))\cdot d_2(v/T^{1-+}(G)) + \sum_{v\in E(G)} d_1(v/T^{1-+}(G))\cdot d_2(v/T^{1-+}(G)).$$

By using Proposition 2.5(iv), we obtain

$$= \sum_{v\in V(G)} (n-1+d_1(v/G))(m-d_1(v/G)) + \sum_{v\in E(G)} (m+1-d_1(v/G))(n-2+d_1(v/G))$$

$$= 2m^2 + mn(n-1) + (m-n+2)M_1(G) - 2m(m+2) + m(m+1)(n-2) - EM_1(G).$$

Theorem 2.25. *For the graph* $T^{+1+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$LM_1(T^{+1+}(G)) = LM_1(G) + M_1(G) - 2LM_3(G) + (n-4)m^2 + m(n-2)^2 + 2m\sum_{v\in V(G)} d_2(v/G);$$

$$LM_2(T^{+1+}(G)) = LM_2(G) + (m+n-2)LM_3(G) - (m+n-2)M_1(G) + M_2(G) + m^2(2n+m-4)$$

$$+\frac{1}{2}m(m-1)(n-2)^2 - \sum_{v\in V(G)} d_2(v/G) \sum_{u\in N_G(v)} d_1(u/G);$$

$$LM_3(T^{+1+}(G)) = 2(LM_3(G) - M_1(G) + 2m^2) + m(m+1)(n-2).$$

Proof. From Eq. (1.1), we have

$$LM_1(T^{+1+}(G)) = \sum_{v\in V(T^{+1+}(G))} d_2(v/T^{+1+}(G))^2$$

$$= \sum_{v\in V(G)} d_2(v/T^{+1+}(G))^2 + \sum_{e\in E(G)} d_2(e/T^{+1+}(G))^2.$$

By using Proposition 2.5(v), we obtain

$$= \sum_{v\in V(G)} (d_2(v/G) - d_1(v/G) + m)^2 + \sum_{e\in E(G)} (n-2)^2$$

$$= LM_1(G) + M_1(G) - 2LM_3(G) + (n-4)m^2 + m(n-2)^2 + 2m\sum_{v\in V(G)} d_2(v/G).$$

Next, from Eq. (1.2), we have

$$LM_2(T^{+1+}(G)) = \sum_{uv\in E(T^{+1+}(G))} d_2(u/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G))$$

$$= \sum_{uv\in E(G)} d_2(u/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G)) + \sum_{uv\in E(S(G))} d_2(u/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G))$$

$$+\sum_{u,v\in E(G)} d_2(u/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G)).$$

By using Proposition 2.5(v), we obtain

$$= \sum_{uv\in E(G)} (d_2(u/G)-d_1(u/G)+m)(d_2(v/G)-d_1(v/G)+m)$$

$$+\sum_{uv\in E(S(G))} (d_2(u/G)-d_1(u/G)+m)(n-2) + \sum_{u,v\in E(G)} (n-2)^2$$

$$= LM_2(G)+(m+n-2)LM_3(G)-(m+n-2)M_1(G)+M_2(G)+m^2(2n+m-4)$$

$$+\frac{1}{2}m(m-1)(n-2)^2 - \sum_{v\in V(G)} d_2(v/G)\sum_{u\in N_G(v)} d_1(u/G).$$

Now, from Eq. (1.3) and the fact that $d_1(v/T^{+1+}(G)) = \begin{cases} 2d_1(v/G) & if\ v\in V(G), \\ m+1 & if\ v\in E(G), \end{cases}$ we have

$$LM_3(T^{+1+}(G)) = \sum_{v\in V(T^{+1+}(G))} d_1(v/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G))$$

$$= \sum_{v\in V(G)} d_1(v/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G)) + \sum_{v\in E(G)} d_1(v/T^{+1+}(G))\cdot d_2(v/T^{+1+}(G)).$$

By using Proposition 2.5(v), we obtain

$$= \sum_{v\in V(G)} 2d_1(v/G)(d_2(v/G)-d_1(v/G)+m) + \sum_{v\in E(G)} (m+1)(n-2)$$

$$= 2(LM_3(G)-M_1(G)+2m^2)+m(m+1)(n-2).$$

Theorem 2.26. *For the graph* $T^{01+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$LM_1(T^{01+}(G)) = nm^2+m(n-2)^2;$$

$$LM_2(T^{01+}(G)) = \frac{1}{2}m(n-2)(2m-n+mn+2);$$

$$LM_3(T^{01+}(G)) = m(mn+n-2).$$

Proof. From Eq. (1.1), we have

$$\begin{aligned} LM_1(T^{01+}(G)) &= \sum_{v\in V(T^{01+}(G))} d_2(v/T^{01+}(G))^2 \\ &= \sum_{v\in V(G)} d_2(v/T^{01+}(G))^2 + \sum_{e\in E(G)} d_2(e/T^{01+}(G))^2. \end{aligned}$$

By using Proposition 2.5(vi), we obtain

$$\begin{aligned} &= \sum_{v\in V(G)} m^2 + \sum_{e\in E(G)} (n-2)^2 \\ &= nm^2 + m(n-2)^2. \end{aligned}$$

From Eq. (1.2), we have

$$\begin{aligned} LM_2(T^{01+}(G)) &= \sum_{uv\in E(T^{01+}(G))} d_2(u/T^{01+}(G))\cdot d_2(v/T^{01+}(G)) \\ &= \sum_{uv\in E(S(G))} d_2(u/T^{01+}(G))\cdot d_2(v/T^{01+}(G)) + \sum_{u,v\in E(G)} d_2(u/T^{01+}(G))\cdot d_2(v/T^{01+}(G)). \end{aligned}$$

By using Proposition 2.5(vi), we obtain

$$\begin{aligned} &= \sum_{uv\in E(S(G))} m(n-2) + \sum_{u,v\in E(G)} (n-2)^2 \\ &= \frac{1}{2} m(n-2)(2m-n+mn+2). \end{aligned}$$

Now, from Eq. (1.3) and the fact that $d_1(v/T^{01+}(G)) = \begin{cases} d_1(v/G) & if\ v\in V(G), \\ m+1 & if\ v\in E(G), \end{cases}$ we have

$$\begin{aligned} LM_3(T^{01+}(G)) &= \sum_{v\in V(T^{01+}(G))} d_1(v/T^{01+}(G))\cdot d_2(v/T^{01+}(G)) \\ &= \sum_{v\in V(G)} d_1(v/T^{01+}(G))\cdot d_2(v/T^{01+}(G)) + \sum_{v\in E(G)} d_1(v/T^{01+}(G))\cdot d_2(v/T^{01+}(G)). \end{aligned}$$

By using Proposition 2.5(vi), we obtain

$$\begin{aligned} &= \sum_{v\in V(G)} (d_1(v/G))m + \sum_{v\in E(G)} (m+1)(n-2) \\ &= m(mn+n-2). \end{aligned}$$

The proof of the following theorems are analogous to that of the above.

Theorem 2.27. *For the graph* $T^{-0+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$\begin{aligned}
LM_1(T^{-0+}(G)) &= \sum_{v\in V(G)} D_3(v/G)^2 - 2m\sum_{v\in V(G)} D_3(v/G) + \sum_{e\in E(G)} \overline{D_2}(e/G)^2 - 4(n-2)\sum_{e\in E(G)} \overline{D_2}(e/G)\\
&\quad + m(4n^2+mn-16n+16);\\
LM_2(T^{-0+}(G)) &= \frac{1}{2}m^2(n^2+7n-2m-16) - m\sum_{uv\notin E(G)}(D_3(u/G)+D_3(v/G))\\
&\quad + \sum_{uv\notin E(G)} D_3(u/G)\cdot D_3(v/G) - 2m\sum_{e\in E(G)} \overline{D_2}(e/G) - 2(n-2)\sum_{v\in V(G)} d_1(v/G)D_3(v/G)\\
&\quad + \sum_{v\in V(G), e\in E(G), v\sim e} D_3(v/G)\overline{D_2}(e/G);\\
LM_3(T^{-0+}(G)) &= m(n^2+3n-8) - (n-1)\sum_{v\in V(G)} D_3(v/G) - 2\sum_{e\in E(G)} \overline{D_2}(e/G).
\end{aligned}$$

Theorem 2.28. *For the graph* $T^{1++}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$\begin{aligned}
LM_1(T^{1++}(G)) &= nm^2 + M_1(G) - 4m^2 + m(n-2)^2 + LM_1(L(G))\\
&\quad + 2(n-2)\sum_{e\in E(G)}\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G));\\
LM_2(T^{1++}(G)) &= \frac{1}{2}nm^2(n-1) + \frac{1}{2}(n^2-6n+7)M_1(G) - m(n-2)^2 + (n-2)LM_3(L(G))\\
&\quad + LM_2(L(G)) + 2m\sum_{e\in E(G)}\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G))\\
&\quad + \sum_{v\in V(G), e\in E(G), v\sim e} d_1(v/G)\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G));\\
LM_3(T^{1++}(G)) &= mn(n-1) + 2m(m-n+1) + (n-3)M_1(G)\\
&\quad + \sum_{e\in E(G)}(2+d_1(e/G))\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G)).
\end{aligned}$$

Theorem 2.29. *For the graph* $T^{-++}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$\begin{aligned}
LM_1(T^{-++}(G)) &= nm^2 + m(n-2)^2 + LM_1(L(G))\\
&\quad + 2(n-2)\sum_{e\in E(G)}\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G));\\
LM_2(T^{-++}(G)) &= \frac{1}{2}m^2(n^2+3n-8) - m^3 - m(n-2)^2 + \frac{1}{2}(n-2)^2M_1(G) + (n-2)LM_3(L(G))\\
&\quad + LM_2(L(G)) + 2m\sum_{e\in E(G)}\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G));\\
LM_3(T^{-++}(G)) &= mn(n-1) + (n-2)M_1(G)\\
&\quad + \sum_{e\in E(G)}(2+d_1(e/G))\sum_{z\in(N_G(u)\cup N_G(v))}(d_1(z/G)-1)-(D_1(e/G)+D_2(e/G)).
\end{aligned}$$

Theorem 2.30. *For the graph* $T^{0-+}(G)$ *of a graph* G *, the leap Zagreb indices are given by*

$$\begin{aligned}
LM_1(T^{0-+}(G)) &= (2n-3)M_1(G)+EM_1(G)-3m(n-2)+\sum_{v\in V(G)}\overline{D_4}(v/G)+\sum_{v\in V(G)}d_1(v/G)\overline{D_4}(v/G);\\
LM_2(T^{0-+}(G)) &= \frac{1}{2}m(m+1)(n-2)^2+\frac{1}{2}(n^2-6n+12)M_1(G)+2M_2(G)+F(G)+(n-2)\overline{EM_1}(G)\\
&\quad+\overline{EM_2}(G)+(n-2)\sum_{v\in V(G)}d_1(v/G)\overline{D_4}(v/G)+\sum_{v\in V(G)}d_1(v/G)\overline{D_4}(v/G)\\
&\quad+\sum_{v\in V(G),e\in E(G),v\sim e}\overline{D_4}(v/G)d_1(e/G);\\
LM_3(T^{0-+}(G)) &= m(3n-4m+mn-8)-(n-m-4)M_1(G)-EM_1(G)+\sum_{v\in V(G)}d_1(v/G)\overline{D_4}(v/G).
\end{aligned}$$

Theorem 2.31. *For the graph* $T^{+-+}(G)$ *of a graph* G, *the leap Zagreb indices are given by*

$$\begin{aligned}
LM_1(T^{+-+}(G)) &= 4LM_1(G)+2(n-2)M_1(G)+EM_1(G)+5m(n-2)+\sum_{v\in V(G)}\overline{D_4}(v/G)\\
&\quad+4\sum_{v\in V(G)}d_2(v/G)\overline{D_4}(v/G);\\
LM_2(T^{+-+}(G)) &= 4LM_2(G)+2(n-2)LM_3(G)-\frac{1}{2}(n-2)^2M_1(G)+(n-2)\overline{EM_1}(G)+\overline{EM_2}(G)\\
&\quad+2\sum_{uv\in E(G)}(d_2(u/G)\overline{D_4}(v/G)+d_2(v/G)\overline{D_4}(u/G))+\sum_{uv\in E(G)}\overline{D_4}(u/G)\overline{D_4}(v/G)\\
&\quad+2\sum_{v\in V(G),e\in E(G),v\sim e}d_2(v/G)d_1(e/G)+(n-2)\sum_{v\in V(G)}d_1(v/G)\overline{D_4}(v/G)\\
&\quad+\sum_{v\in V(G),e\in E(G),v\sim e}\overline{D_4}(v/G)d_1(e/G)+\frac{1}{2}m(m+1)(n-2)^2;\\
LM_3(T^{+-+}(G)) &= 4LM_3(G)+(m-n+3)M_1(G)-EM_1(G)+m(3n-2m+mn-6)\\
&\quad+\sum_{v\in V(G)}d_1(v/G)\overline{D_4}(v/G).
\end{aligned}$$

Theorem 2.32. *For the graph* $T^{--+}(G)$ *of a graph* G, *the leap Zagreb indices are given by*

$$\begin{aligned}
LM_1(T^{--+}(G)) &= nm(n+m-2)+M_1(G);\\
LM_2(T^{--+}(G)) &= \frac{1}{2}m^2(n^2+3n-16)-m^3-\frac{1}{2}(n^2-4n-4m+4)M_1(G)+(n-2)\overline{EM_1}(G)\\
&\quad+\overline{EM_2}(G)+\frac{1}{2}m(m+1)(n-2)^2;\\
LM_3(T^{--+}(G)) &= m(n^2+2n-4m+mn-8)+(m-n+3)M_1(G)-EM_1(G).
\end{aligned}$$

ACKNOWLEDGEMENT

[*] This work is partially supported by the University Grants Commission (UGC), New Delhi, through UGC-SAP DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I) dated: 29th Feb. 2016.

[1] This work is supported by Directorate of Minorities, Banglore, Fellowship: Ph. D/M. Phil - 2017-18, No. DOM/FELLOWSHIP/CR-29/2017-18 dated: 09th Aug. 2017.

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Int. J. Math. And Appl., 6(2–B)(2018), 141–150

ISSN: 2347-1557

Available Online: http://ijmaa.in/

International Journal of *Mathematics And its Applications*

Computing First Leap Zagreb Index of Some Nano Structures

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Abstract: Topological indices have several chemical applications in the quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis of chemical compounds. In this paper, we study the linear regression analysis of the first leap Zagreb index with respect to entropy, acentric factor, enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) and boiling point of octane isomers. Finally, we present the expressions for first leap Zagreb index of certain nano structures.

MSC: 05C90, 05C35, 05C12.

Keywords: First Zagreb index, leap Zagreb index, line graph, subdivision graph, line graph.

Accepted on: 19.04.2018

1. Introduction

Let $G = (n, m)$ be a simple graph with vertex set V and edge set E. The *k-neighborhood* [13] of a vertex $v \in V(G)$, denoted by $N_k(v/G)$, and $N_k(v/G) = \{u \in V(G) : d(u, v) = k\}$ in which $d(u, v)$ is the distance between the vertices u and v in G, i.e., the length of the shortest path joining u and v in G. The *k-distance degree of a vertex* $v \in V(G)$, denoted by $d_k(v/G)$, and $d_k(v/G) = |N_k(v/G)|$. Also, we denote $N_1(v/G)$ by $N_G(v)$ and $d_1(v/G)$ by $d_G(v)$. The *degree of an edge* $e = uv$ in G, denoted by $d_1(e/G)$ (or $d_G(e)$), is defined by $d_1(e/G) = d_1(u/G) + d_1(v/G) - 2$. If all the vertices of G have same degree equal to $r \in Z^+$, then G is called a r-regular graph. The subdivision graph of a graph G, denoted by $S(G)$, is the graph obtained from G by inserting a new vertex of degree two on each of its edge [8]. The line graph of a graph G, denoted by $L(G)$, is the graph with vertex set $E(G)$ and two vertices in $L(G)$ are adjacent if and only if they correspond to two adjacent edges in G [8]. For unexplained graph terminology and notation refer [8].

The physico-chemical properties of a molecule can be easily studied by graph invariants associated with the graphs corresponding to the chemical molecule. One of such graph invariants is topological index. Recently in [12], Naji et al. has introduced a novel topological index called first leap Zagreb index which is defined as the sum of squares of *2-distance degree* of vertices of a graph G, denoted by $LM_1(G)$, i.e., $LM_1(G) = \sum_{v \in V(G)} (d_2(v/G))^2$. There are plenty of topological indices defined in the literature. Zagreb indices[7], F-index[6], connectivity index (or Randić index) [5] are few of them. Very recently indices like Sanskruti index[9], second order first Zagreb index [2] and (β, α)-connectivity index [3] are introduced. Since it is higher order topological index and it has advanced chemical applications in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) study.

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In [12], Naji et al. have left to identify the chemical applications of first leap Zagreb index. Surprisingly, this index has very good correlation with physical properties of chemical compounds like boiling point, entropy, DHVAP, HVAP and accentric factor. Therefore, we present here a linear regression model of these physical properties with first leap Zagreb index.

In the present work, we consider 2D-Lattice, nanotube, nanotorus of $TUC_4C_8[p,q]$. Let p and q denote the number of squares in a row and the number of rows of squares, respectively in $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$. An example of $2D$-lattice, nanotube and nanotorus of $TUC_4C_8[4,3]$ is given in Fig. 1 (a), (b) and (c) respectively. Recently in [1, 2, 9–11], authors obtained the expressions for certain topological indices of line graph of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$.

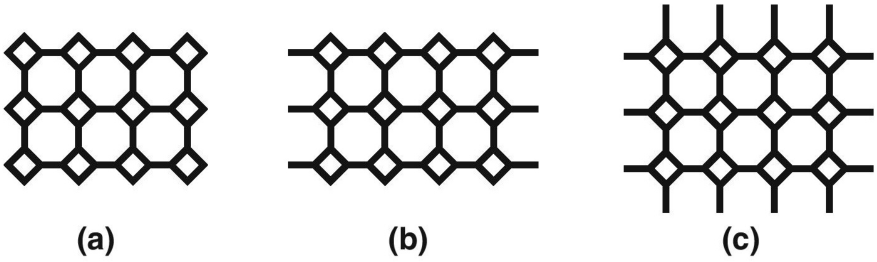

Figure 1. **(a) 2D-lattice of $TUC_4C_8[4,3]$; (b) $TUC_4C_8[4,3]$ nanotube; (c) $TUC_4C_8[4,3]$ nanotorus.**

The present work is organized as follows; In Section 2, we study the chemical applicability of the first leap Zagreb index. In Sections 3 and 4, we obtain explicit formulae for computing the first leap Zagreb index of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ together with those of line graphs of subdivision graphs of 2D-lattice, nanotube and nanotorus of $TUC_4C_8[p,q]$ respectively.

2. On chemical applicability of the first leap Zagreb index

The topological indices with the higher correlation factor are of foremost important in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis. In this section we discuss the linear regression analysis of first leap Zagreb index with entropy(S), acentric factor(AcentFac), enthalpy of vaporization (HVAP), standard enthalpy of vaporization (DHVAP) and boiling point(BP) of octane isomers on the degree based topological indices of the corresponding molecular graph. The first leap Zagreb index was tested using a dataset of octane isomers found at http://www.moleculardiscriptors.eu/dataset.htm. The dataset of octane isomers(columns 1-6 of Table 1) are taken from above web link whereas last column of Table 1 is computed by definition of first leap Zagreb index.

Alkane	BP	S	AcentFac	DHVAP	HVAP	LM_1
n-octane	125.665	111.67	0.397898	9.915	73.19	20
2-methyl-heptane	117.647	109.84	0.377916	9.484	70.3	28
3-methyl-heptane	118.925	111.26	0.371002	9.521	71.3	28
4-methyl-heptane	117.709	109.32	0.371504	9.483	70.91	30
3-ethyl-hexane	118.534	109.43	0.362472	9.476	71.7	30
2,2-dimethyl-hexane	106.84	103.42	0.339426	8.915	67.7	50
2,3-dimethyl-hexane	115.607	108.02	0.348247	9.272	70.2	36
2,4-dimethyl-hexane	109.429	106.98	0.344223	9.029	68.5	48
2,5-dimethyl-hexane	109.103	105.72	0.35683	9.051	68.6	36
3,3-dimethyl-hexane	111.969	104.74	0.322596	8.973	68.5	50
3,4-dimethyl-hexane	117.725	106.59	0.340345	9.316	70.2	36
2-methyl-3-ethyl-pentane	115.45	106.06	0.332433	9.209	69.7	38

Alkane	BP	S	AcentFac	DHVAP	HVAP	LM_1
3-methyl-3-ethyl-pentane	118.259	101.48	0.306899	9.081	69.3	48
2,2,3-trimethyl-pentane	109.841	101.31	0.300816	8.826	67.3	56
2,2,4-trimethyl-pentane	99.238	104.09	0.30537	8.402	64.87	62
2,3,3-trimethyl-pentane	114.76	102.06	0.293177	8.897	68.1	54
2,3,4-trimethyl-pentane	113.467	102.39	0.317422	9.014	68.37	44
2,2,3,3-tetramethylbutane	106.47	93.06	0.255294	8.41	66.2	72

Table 1. Experimental values of the entropy, acentric factor, HVAP, DHVAP, boiling point and the corresponding value of first leap Zagreb index of octane isomers.

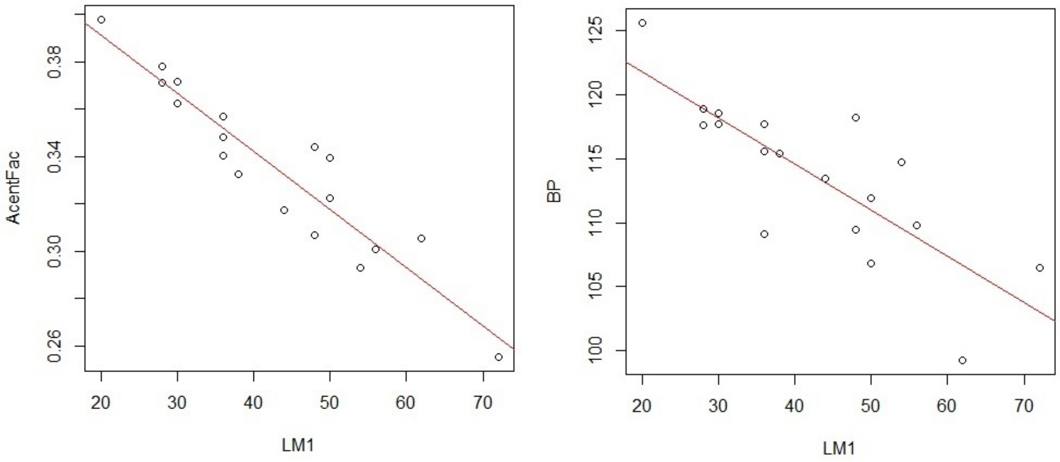

Figure 2. **Scatter diagram of (a) $AcentFac$ on LM_1, (b) BP on LM_1 superimposed by the fitted regression line.**

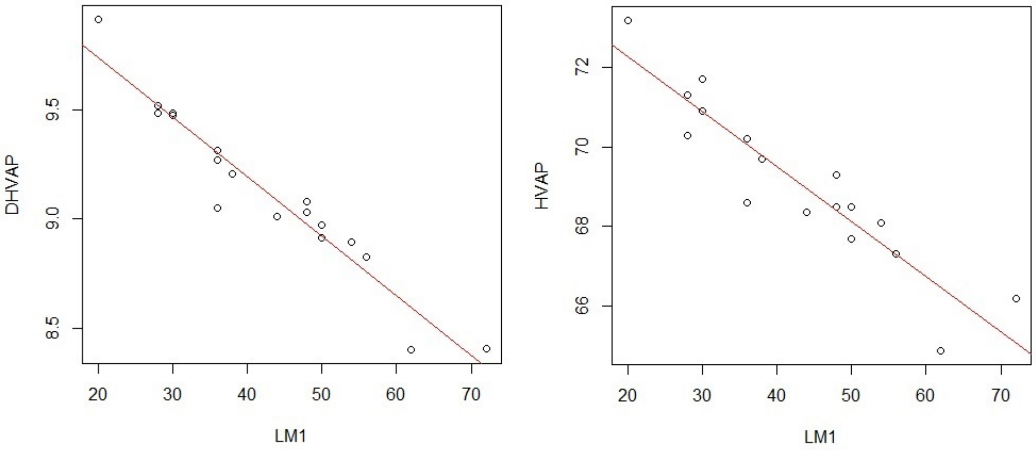

Figure 3. **Scatter diagram of (a) $DHVAP$ on LM_1 (b) $HVAP$ on LM_1, super imposed by the fitted regression line.**

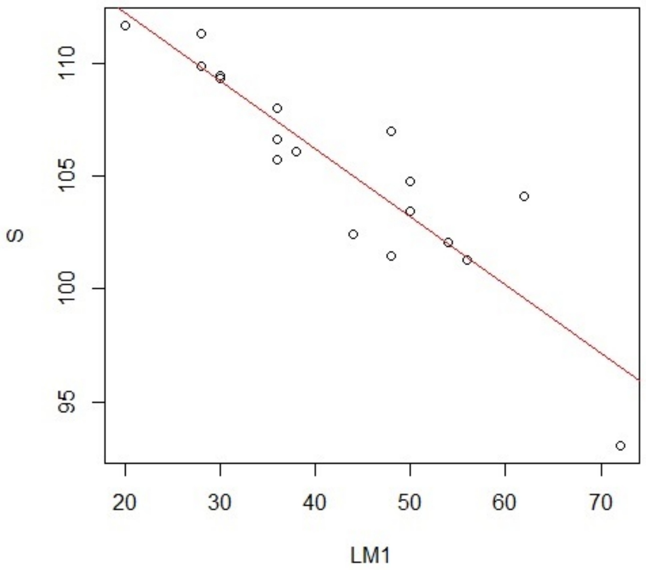

Figure 4. **Scatter diagram of (a) S on LM_1, super imposed by the fitted regression line.**

The linear regression models for the entropy, acentric factor, DHVAP, HVAP and boiling point using the data of Table 1 are obtained using the least squares fitting procedure as implemented in R software [4]. The fitted models are:

$$\hat{S} = 118.20831(\pm 1.59739) - 0.30067(\pm 0.03586)LM_1 \tag{1}$$

$$Acent\hat{F}ac = 0.4402084(\pm 0.0100259) - 0.0024542(\pm 0.0002251)LM_1 \tag{2}$$

$$DH\hat{V}AP = 10.285778(\pm 0.083792) - 0.027245(\pm 0.001881)LM_1 \tag{3}$$

$$H\hat{V}AP = 75.04885(\pm 0.62979) - 0.13830(\pm 0.01414)LM_1 \tag{4}$$

$$\hat{B}P = 129.05174(\pm 3.01640) - 0.36070(\pm 0.06771)LM_1 \tag{5}$$

Note: The values in the brackets of Equations (1) to (5) are the corresponding standard errors of the regression coefficients. The index is better as $|r|$ approaches 1.

Physical Property	Absolute value of the correlation coefficient ($\lvert r \rvert$)	Residual standard error
Entropy	0.9025673	2.005
Acentric Factor	0.9388335	0.01258
DHVAP	0.9639245	0.1052
HVAP	0.9256201	0.7904
BP	0.7996668	3.786

Table 2. **Correlation coefficient and residual standard error of regression models**

From Table 2, we can observe that LM_1 correlates highly with DHVAP with the correlation coefficient $|r| = 0.9639245$. The most interesting observation is that it has more correlation with boiling point as compared to that of Wiener index. Also LM_1 has good correlation ($|r| > 0.9$) with entropy, accentric factor, DHVAP and HVAP.

3. First Leap Zagreb Index of 2D-lattice, Nanotube and Nanotorus of $TUC_4C_8[p,q]$

Graph	Order	Size
2D-Lattice of $TUC_4C_8[p,q]$	$4pq$	$6pq-p-q$
$TUC_4C_8[p,q]$ Nanotube	$4pq$	$6pq-p$
$TUC_4C_8[p,q]$ Nonotorus	$4pq$	$6pq$

Table 3. **Order and Size of graphs**

$d_2(v/A)$	2	3	4	5
Number of Vertices	8	$2(p+q-4)$	4(p+q-2)	$2(2pq-3p-3q+4)$

Table 4. **Vertex partition of the Graph A when $p>1, q>1$**

$d_2(v/A)$	1	2	3
Number of Vertices	2	4	$2(2p-3)$

Table 5. **Vertex partition of the Graph A when $p>1, q=1$**

Theorem 3.1. *Let A be a $2D$-lattice of $TUC_4C_8[p,q]$. Then*

$$LM_1(A)=\begin{cases} 4(25pq-17p-17q+8) & if\ p>1, q>1 \\ 36(p-1) & if\ p>1, q=1. \end{cases}$$

Proof. The $2D$-lattice of $TUC_4C_8[p,q]$ has $4pq$ vertices and $6pq-p-q$ edges. Therefore, we can partition the vertex set of A into the following cases:

Case 1: when $p>1$ and $q>1$. From the Table 4, we can see that the vertex partition is obtained based on the *2-distance degree* of each vertex. Now,

$$\begin{aligned} LM_1(A) &= \sum_{v\in V(A)} (d_2(v/A))^2 \\ &= 8\times(2)^2+2(p+q-4)\times 3^2+4(p+q-2)\times 4^2+2(2pq-3p-3q+4)\times 5^2 \\ &= 4(25pq-17p-17q+8). \end{aligned}$$

Case 2: when $p>1$ and $q=1$. The vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 5. Now,

$$\begin{aligned} LM_1(A) &= \sum_{v\in V(A)} (d_2(v/A))^2 \\ &= 2\times(1)^2+4\times 2^2+2(2p-3)\times 3^2 = 36(p-1). \end{aligned}$$

□

$d_2(v/B)$	3	4	5
Number of Vertices	$2p$	$4p$	$2p(2q-3)$

Table 6. **Vertex partition of the Graph B when $p>1, q>1$**

$d_2(v/B)$	3
Number of Vertices	$4p$

Table 7. **Vertex partition of the Graph B when $p > 1, q = 1$**

Theorem 3.2. *Let B be a $TUC_4C_8[p,q]$ nanotube. Then*

$$LM_1(B)=\begin{cases} 4p(25q-17) & if\ p>1, q>1 \\ 36p & if\ p>1, q=1. \end{cases}$$

Proof. The $TUC_4C_8[p,q]$ nanotube has $4pq$ vertices and $6pq-p$ edges. Therefore, we can partition the vertex set of B into the following cases:

Case 1: when $p > 1$ and $q > 1$. From the Table 6, we can see that the vertex partition is obtained based on the *2-distance degree* of each vertex. Now,

$$\begin{aligned} LM_1(B) &= \sum_{v\in V(B)} (d_2(v/B))^2 \\ &= 2p\times 3^2 + 4p\times 4^2 + 2p(2q-3)\times 5^2 \\ &= 4p(25q-17). \end{aligned}$$

Case 2: when $p > 1$ and $q = 1$, the vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 7. Now,

$$\begin{aligned} LM_1(B) &= \sum_{v\in V(B)} (d_2(v/B))^2 \\ &= 4p\times 3^2 \\ &= 36p. \end{aligned}$$

□

Table 8. **Vertex partition of the Graph C**

$d_2(v/C)$	5
Number of Vertices	$4pq$

Theorem 3.3. *Let C be a $TUC_4C_8[p,q]$ nanotorus. Then $LM_1(C) = 100pq$.*

Proof. The $TUC_4C_8[p,q]$ nanotorus is shown in Fig. 1. The graph C is 3-regular with $4pq$ vertices and has *2-distance degree* of each vertex as 5. Therefore,

$$\begin{aligned} LM_1(C) &= \sum_{v\in V(C)} (d_2(v/C))^2 \\ &= 4pq\times 5^2 \\ &= 100pq. \end{aligned}$$

□

4. First Leap Zagreb Index of Line Graph of Subdivision Graphs of 2D-lattice, Nanotube and Nanotorus of $TUC_4C_8[p,q]$

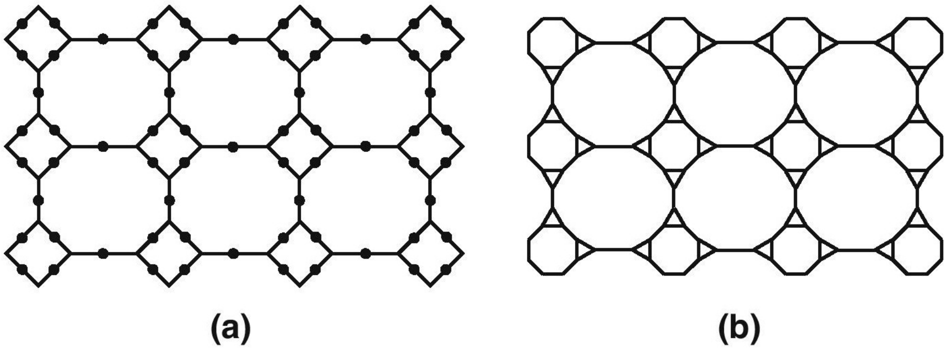

Figure 5. (a) Subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$; (b) line graph of the subdivision graph of 2D-lattice of $TUC_4C_8[4,3]$.

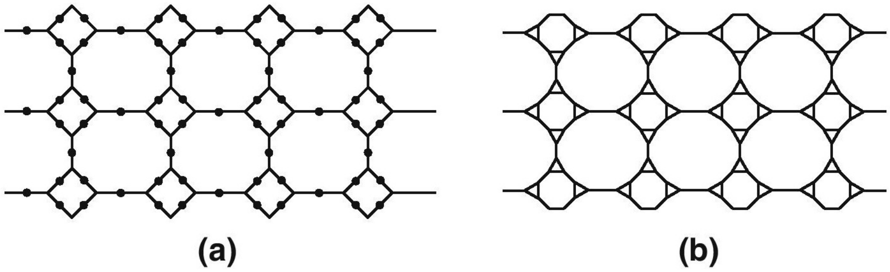

Figure 6. (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotube; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotube.

$d_2(v/A_1)$	2	3	4
Number of Vertices	8	$4pq$	$2(4pq-p-q-4)$

Table 9. **Vertex partition of the Graph A_1 when $p>1, q>1$**

$d_2(v/A_1)$	2	3	4
Number of Vertices	8	$8(p-1)$	$2(p-1)$

Table 10. **Vertex partition of the Graph A_1 when $p>1, q=1$**

Theorem 4.1. *Let A_1 be a line graph of the subdivision graph of $2D$-lattice of $TUC_4C_8[p,q]$. Then*

$$LM_1(A_1)=\begin{cases}164pq-32p-32q-96 & if\ p>1, q>1\\ 8(13p-9) & if\ p>1, q=1.\end{cases}$$

Proof. The $2D$-lattice of $TUC_4C_8[p,q]$ has $4pq$ vertices and $6pq-p-q$ edges. The subdivision graph of $2D$-lattice of $TUC_4C_8[p,q]$ has $10pq-p-q$ vertices and $2(6pq-p-q)$ edges. Thus, line graph of subdivision graph of $2D$-lattice of $TUC_4C_8[p,q]$ has vertices $2(6pq-6-q)$ and $18pq-5p-5q$ edges. Therefore, we can partition the vertex set of A_1 into the following cases:

Case 1: When $p>1$ and $q>1$. From the Table 9, we can see that the vertex partition is obtained based on the *2-distance* *degree* of each vertex. Now,

$$\begin{aligned} LM_1(A_1) &= \sum_{v\in V(A_1)} (d_2(v/A_1))^2 \\ &= 8\times(2)^2 + 4pq\times 3^2 + 2(4pq-p-q-4)\times 4^2 \\ &= 164pq - 32p - 32q - 96. \end{aligned}$$

Case 2: When $p > 1$ and $q = 1$. The vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 10. Now,

$$\begin{aligned} LM_1(A_1) &= \sum_{v\in V(A_1)} (d_2(v/A_1))^2 \\ &= 8\times(2)^2 + 8(p-1)\times 3^2 + 2(p-1)\times 4^2 \\ &= 8(13p-9). \end{aligned}$$

□

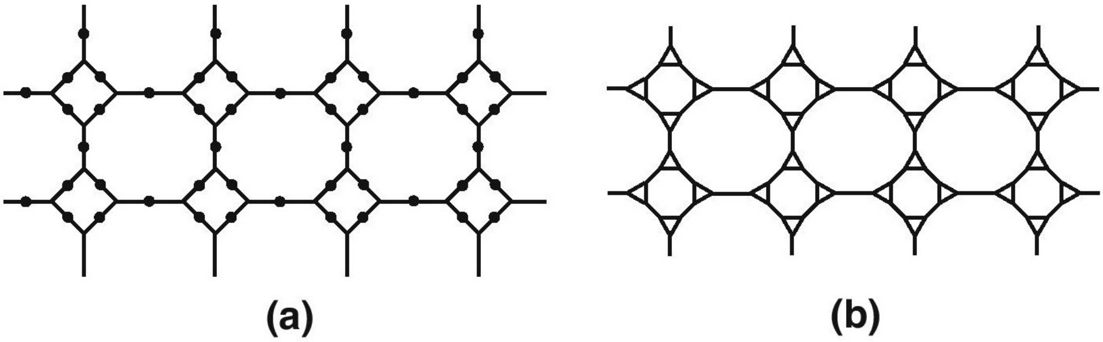

Figure 7. (a) Subdivision graph of $TUC_4C_8[4,3]$ of nanotorus; (b) line graph of the subdivision graph of $TUC_4C_8[4,3]$ of nanotorus.

$d_2(v/B_1)$	3	4
Number of Vertices	$8p$	$2p(6q-5)$

Table 11. Vertex partition of the Graph B_1 when $p > 1, q > 1$

$d_2(v/B_1)$	3	4
Number of Vertices	$8p$	$2p$

Table 12. Vertex partition of the Graph B_1 when $p > 1, q = 1$

Theorem 4.2. *Let B_1 be a line graph of the subdivision graph of $TUC_4C_8[p,q]$ nanotube. Then*

$$LM_1(B_1)=\begin{cases} 8p(24q-11) & if\ p>1, q>1 \\ 104p & if\ p>1, q=1. \end{cases}$$

Proof. The $TUC_4C_8[p,q]$ nanotube has $4pq$ vertices and $6pq-p$ edges. The subdivision graph of $TUC_4C_8[p,q]$ nanotube has $10pq-p$ vertices and $12pq-2p$ edges. Thus line graph of subdivision graph of $TUC_4C_8[p,q]$ nanotube has $12pq-2p$ vertices and $18pq-5p$ edges. Therefore, we can partition the vertex set of B_1 into the following cases:

Case 1: When $p > 1$ and $q > 1$. From the Table 11, we can see that the vertex partition is obtained based on the *2-distance degree* of each vertex. Now,

$$\begin{aligned} LM_1(B_1) &= \sum_{v \in V(B_1)} (d_2(v/B_1))^2 \\ &= 8p \times 3^2 + 2p(6q-5) \times 4^2 \\ &= 8p(24q-11). \end{aligned}$$

Case 2: When $p > 1$ and $q = 1$, the vertex partition is obtained on the base of the *2-distance degree* of each vertex which is shown in Table 12. Now,

$$\begin{aligned} LM_1(B_1) &= \sum_{v \in V(B_1)} (d_2(v/B_1))^2 \\ &= 8p \times 3^2 + 2p \times 4^2 \\ &= 104p. \end{aligned}$$

□

Table 13. **Vertex partition of Graph C_1**

$d_2(v/C_1)$	4
Number of Vertices	$12pq$

Theorem 4.3. *Let C_1 be a line graph of the subdivision graph of $TUC_4C_8[p,q]$ of nanotorus. Then $LM_1(C_1) = 192pq$.*

Proof. The subdivision graph of $TUC_4C_8[p,q]$ of nanotorus and the graph C_1 are shown in Fig. 7 (a) and (b). The graph C_1 is 3-regular with $12pq$ vertices and has *2-distance degree* of each vertex as 4. Therefore,

$$\begin{aligned} LM_1(C_1) &= \sum_{v \in V(C_1)} (d_2(v/C_1))^2 \\ &= 12pq \times 4^2 \\ &= 192pq. \end{aligned}$$

□

Acknowledgement

* This work is partially supported by the University Grants Commission (UGC), New Delhi, through UGC-SAP DRS-III for 2016-2021: F.510/3/DRS-III/2016(SAP-I).

[1] This work is supported by Directorate of Minorities Fellowship: Ph. D/M. Phil - 2017-18, No. DOM/FELLOWSHIP/CR-29/2017-18.

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International Journal of Advance Research in Science and Engineering
Volume No.07, Special Issue No.(02), March 2018
www.ijarse.com
IJARSE
ISSN: 2319-8354

A Study of Some Topological Indices of Grid

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ABSTRACT

In this paper, computation of the Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index and SK_2 index of grid is carried out without the aid of acomputer.

Keywords: Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2 index and grid.

I.INTRODUCTION

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [3, 4]. This theory had an important effect on the development of the chemical sciences.

In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [4].

Let $G= (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [1].

II. COMPUTING THE TOPOLOGICAL INDICES OF GRID.

Motivated by previous research on grid, here we used to four new topological indices and computed their corresponding topological index value of grid [6].

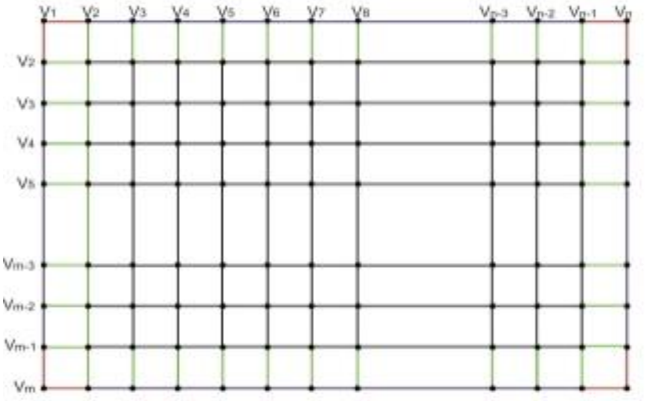

Figure 1

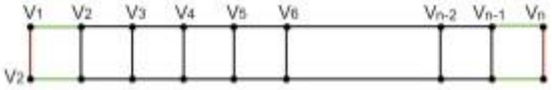

Figure 2

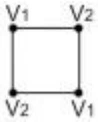

Figure 3

In [5,7,8,9 and 10], Shigehalli and Kanabur have put forward new degree based topological indices viz. arithmetic-geometric index, SK index, SK_1 index and SK_2 index. Which are defined as follows:

Definition 2.1: Arithmetic-Geometric (AG_1) Index

Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u, then AG_1 index of G is defined as

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

Where, AG_1index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

Definition 2.2: *SK* Index

The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.3: SK_1 Index

The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

Definition 2.4: ***SK_2* Index**

The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

III.MAIN RESULTS

Theorem3.1: The AG_1 index of grid with *"(m-1)"* rows and *"(n-1)"*columns is given by

$$AG_1(G) = \begin{cases} 2mn - 0.9793m - 0.9793n - 8.0829, & if\ m \succ 2\ and\ n \succ 2 \\ 3n - 1.9174, & if\ m = 2\ and\ n \succ 2 \\ 4, & if\ m = n = 2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by $G(m, n)$, is defined as the Cartesian product $P_m \times P_n$ of undirected pathsP_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

Consider a two-dimensional structure of grid with $(m-1)$ rows and $(n-1)$ columns as shown in the figure1. Let $e_{i,j}$ denotes the number of edges connecting the vertices of degrees d_i and d_j.

Table1.

Row	**$e_{2,3}$**	**$e_{3,3}$**	**$e_{3,4}$**	**$e_{4,4}$**
1	4	n-3	n	n-3
2	0	2	2	2n-5
3	0	2	2	2n-5
4	0	2	2	2n-5
. . .	. . .	. . .	. . .	. . .
m-2	0	2	2	2n-5
m-1	4	n-3	n-2	0
Total	**8**	**2m+2n-12**	**2m+2n-8**	**2mn-5m-5n+12**

Table2.

Row	**$e_{2,2}$**	**$e_{2,3}$**	**$e_{3,3}$**
1	2	4	(3n-8)

$$AG_1(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

$$AG_1(G) = e_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right) + e_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right) + e_{3,4}\left(\frac{3+4}{2\sqrt{3.4}}\right) + e_{4,4}\left(\frac{4+4}{2\sqrt{4.4}}\right)$$

$$=8\left(\frac{5}{2\sqrt{6}}\right) + (2m+2n-12)\,(1) + (2m-2n-8)\left(\frac{7}{2\sqrt{12}}\right) + (2mn-5m-5n+12)\,(1)$$

$$= \frac{20}{\sqrt{6}} + 2m+2n-12 + (m+n-4)\frac{7}{\sqrt{12}} + 2mn-5m-5n+12$$

$$=2mn-3m-3n+\frac{7m}{\sqrt{12}}+\frac{7n}{\sqrt{12}}-\frac{28}{\sqrt{12}}$$

$$= 2mn-0.979m-0.979n-8.0829.$$

Now, we consider the following cases:

Case 1. Ifm>2 and n>2, Grid contains$e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$edges in each row is mentioned in the following table1.

The Arithmetic-Geometric index of grid for if m>2 and n>2

$AG_1(G)$= 2mn-0.979m-0.979n-8.0829

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$,and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$,and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$,and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m=2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$AG_1\,(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

$$AG_1(G) = e_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right) + e_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right) + e_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right)$$

$$= 2\,(1) + 4\left(\frac{5}{2\sqrt{6}}\right) + (3n-8)\,(1)$$

$$= 2 + \frac{20}{\sqrt{6}} + 3n - 8$$

$$= 3n - 1.9174.$$

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$AG_1\,(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

$$AG_1\,(G) = e_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right)$$

$$= 4\,(1)$$

$$= 4.$$

Theorem3.2: The *SK* index of grid with *"(m-1)"* rows of benzene rings and *"(n-1)"* columns is given by

$$SK\,(G) = \begin{cases} 8mn - 7m + 33n + 28, \ if\ m \succ 2\ \ and\ \ n \succ 2 \\ 9n - 10, \ if\ \ m = 2\ \ and\ \ n \succ 2 \\ 8, \ if\ \ m = n = 2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by *G (m, n)*, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

$$SK\,(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$SK\,(G) = e_{2,3}\left(\frac{2+3}{2}\right)+e_{3,3}\left(\frac{3+3}{2}\right)+e_{3,4}\left(\frac{3+4}{2}\right)+e_{4,4}\left(\frac{4+4}{2}\right)$$

$$=8\left(\frac{5}{2}\right)+2\,(m+n-6)\left(\frac{6}{2}\right)+2\,(m+n-4)\left(\frac{7}{2}\right)+(2mn-5m-5n+12)\left(\frac{8}{2}\right)$$

$$= 20+6m+6n-12+7m+7n-28+8mn-20m+20n+48$$

$$= 8mn-7m+33n+28$$

Now, we consider the following cases:

Case 1. If m>2 and n>2, Grid contains $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges in each row is mentioned in the following table1.

The SK index of grid for if m>2 and n>2

$AG_1\,(G)$=8mn-7m+33n+28

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m= 2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$SK\,(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$SK(G) = e_{2,2}\left(\frac{2+2}{2}\right)+e_{2,3}\left(\frac{2+3}{2}\right)+e_{3,3}\left(\frac{3+3}{2}\right)$$

$$=2\left(\frac{4}{2}\right)+4\left(\frac{5}{2}\right)+(3n-8)\left(\frac{6}{2}\right)$$

$$= 4+10+9n-24$$

$= 9n-10.$

Case 3. If *m=n=2*

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2}$$

$$SK(G) = e_{2,2}\left(\frac{2+2}{2}\right)$$

$$=4\left(\frac{4}{2}\right)$$

$= 8.$

Theorem3.3: TheSK_1 index of grid with *“(m-1)”* rows of benzene rings and *“(n-1)”* columns is given by

$$SK_1(G) = \begin{cases} 16mn - 19m + 61n + 18, \; if \; m \succ 2 \; and \; n \succ 2 \\ 13.5n - 20, \; if \; m = 2 \; and \; n \succ 2 \\ 8, \; if \; m = n = 2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by *G (m, n)*, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$SK_1(G) = e_{2,3}\left(\frac{2\times 3}{2}\right) + e_{3,3}\left(\frac{3\times 3}{2}\right) + e_{3,4}\left(\frac{3\times 4}{2}\right) + e_{4,4}\left(\frac{4\times 4}{2}\right)$$

$$=8\left(\frac{6}{2}\right) + 2(m+n-6)\left(\frac{9}{2}\right) + 2(m+n-4)\left(\frac{12}{2}\right) + (2mn-5m-5n+12)\left(\frac{16}{2}\right)$$

$= 24+9m+9n-54+12m+12n-48+16mn-40m+40n+96$

$= 16mn-19m+61n+18.$

Now, we consider the following cases:

Case 1. If m>2 and n>2, Grid contains $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and $e_{4,4}$ edges in each row is mentioned in the following table1.

The SK_1 index of grid for if m>2 and n>2

$SK_1(G)$=16mn-19m+61n+18

Case 2. In this case Grid contains $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges. The edges $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2}$, $e_{2,3}$, and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m = 2$ and $n > 2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

○ $$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$SK_1(G) = e_{2,2}\left(\frac{2\times 2}{2}\right) + e_{2,3}\left(\frac{2\times 3}{2}\right) + e_{3,3}\left(\frac{3\times 3}{2}\right)$$

$$=2\left(\frac{4}{2}\right)+4\left(\frac{6}{2}\right) + (3n-8)\left(\frac{9}{2}\right)$$

$$= 4+12+13.5n-36$$

$$= 13.5n-20.$$

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}$$

$$SK_1(G) = e_{2,2}\left(\frac{2\times 2}{2}\right)$$

$=4\left(\frac{4}{2}\right)$

$= 8.$

Theorem3.4: The*SK₂* index of grid with *“(m-1)”* rows of benzene rings and *“(n-1)”* columns is given by

$$SK_2(G) = \begin{cases} 32mn-37.5m+122.5n+36, \ if \ m \succ 2 \ \ and \ \ n \succ 2 \\ 27n-39, \ if \ \ m=2 \ \ and \ \ n \succ 2 \\ 16, \ if \ \ m=n=2 \end{cases}$$

Proof: The topological structure of a grid network, denoted by *G (m, n)*, is defined as the Cartesian product $P_m \times P_n$ of undirected paths P_m and P_n. The spectrum of the graph does not depends on the numbering of the vertices. However, here we adopt a particular numbering such that the edges has a pattern which is common for any dimension. We follow the sequential numbering from left to right as shown in the figure1.

$$SK_2(G) = \sum_{u,v\in E(G)}\left(\frac{d_G(u)+d_G(v)}{2}\right)^2$$

$$SK_2(G)= e_{2,3}\left(\frac{2+3}{2}\right)^2 + e_{3,3}\left(\frac{3+3}{2}\right)^2 + e_{3,4}\left(\frac{3+4}{2}\right)^2 + e_{4,4}\left(\frac{4+4}{2}\right)^2$$

$$=8\left(\frac{25}{4}\right)+2\,(m+n-6)\left(\frac{36}{4}\right)+2\,(m+n-4)\left(\frac{49}{4}\right)+(2mn-5m-5n+12)\left(\frac{64}{4}\right)$$

$= 50+18m+18n-108+24.5m+24.5n-98+32mn-80m+80n+192$

$= 32mn-37.5m+122.5n+36$

Now, we consider the following cases:

Case 1. If m>2 and n>2, Grid contains $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ only edges. In the figure1 $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ edges are colored in red, blue, green and black respectively. The number of $e_{2,3}$, $e_{3,3}$, $e_{3,4}$ and$e_{4,4}$ edges in each row is mentioned in the following table1.

The SK_2 index of grid for if m>2 and n>2

$AG_1(G)$=32mn-37.5m+122.5n+36

Case 2. In this case Grid contains $e_{2,2,}$ $e_{2,3,}$and $e_{3,3}$ edges. The edges $e_{2,2,}$ $e_{2,3,}$and $e_{3,3}$ are colored in red, blue and black respectively as shown in the figure2. The number of $e_{2,2,}$ $e_{2,3,}$and $e_{3,3}$ edges in each row is mentioned in the table2.

If $m= 2$ and $n>2$

In this case grid contains $e_{2,2}$, $e_{2,3}$ and $e_{3,3}$ edges.

$$SK_2\,(G) = \sum_{u,v\in E(G)} \left(\frac{d_G\left(u\right)+d_G\left(v\right)}{2} \right)^2$$

$$SK_2(G) = e_{2,2}\left(\frac{2+2}{2}\right)^2 + e_{2,3}\left(\frac{2+3}{2}\right)^2 + e_{3,3}\left(\frac{3+3}{2}\right)^2$$

$$= 2\left(\frac{16}{4}\right) + 4\left(\frac{25}{4}\right) + (3n-8)\left(\frac{36}{4}\right)$$

$$= 8+25+27n-72$$

$$= 27n-39.$$

Case 3. If $m=n=2$

In this case the number of $e_{2,2}$ edges is as shown in figure3.

$$SK_2\,(G) = \sum_{u,v\in E(G)} \left(\frac{d_G\left(u\right)+d_G\left(v\right)}{2} \right)^2$$

$$SK_2\,(G) = e_{2,2}\left(\frac{2+2}{2}\right)^2$$

$$= 4\left(\frac{16}{4}\right)$$

$$= 16.$$

IV. CONCLUSION

A generalized formula for Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, SK_2index of Grid is obtained without using computer.

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Journal of Mathematical Nanoscienese 8 (1) (2018) 19–25

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On certain degree-based topological indices of armchair polyhex nanotubes

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Abstract. Recently [18], Shigehalli and Kanabur have introduced two new topological indices namely, AG_2 index and SK_3 index. Hosamani [14], has studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G. In this paper, formula for computing the armchair polyhex nanotube $TUAC_6[m,n]$ family is given.

Keywords. molecular graph, arithmetic-geometric index (AG_2 index), SK_3 index, sanskruti index, armchair polyhex nanotube.

1 Introduction

Let G be a simple connected graph in chemical graph theory. In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [3, 12].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [6, 8, 12]. This theory had an important effect on the development of the chemical sciences.

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DOI: 10.22061/jmns.2017.2897.1022

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_u(G)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [3]. Motivated by previous research on armchair polyhex nanotubes. Here we computed the topological index value of armchair polyhex nanotubes [2,4,7,9,10,11,13,16,17,18].

2 Computing the topological indices of certain nanotubes

The armchair polyhex nanotubes $G = TUAC_6$(Fig. 1) suppose m and n denote the number of hexagons in the first row/column of the 2D-lattice of $TUAC_6[m,n]$ (Fig. 2), respectively. Thus the number of vertices/atoms in this nanotube is equal to $|V(TUAC_6[m,n])| = 2m(n+1)$, $m,n \in E(G)$ and obviously the number of edges/bonds is $|E(TUAC_6[m,n])| = 3mn+2m$.

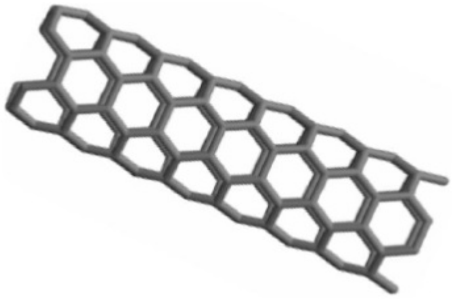

Figure 1. The 3D lattice of Armchair polyhex nanotubes $TUAC_6[m,n]$.

There are two partitions $V_2 = \{v \in V(G)/d_v = 2\}$ and $V_3 = \{v \in V(G)/d_v = 3\}$ of $V(TUAC_6[m,n])$, since the degree of an arbitrary vertex/atom of a molecular graph armchair polyhex is equal to 2 or 3. Next, these partitions imply that $E(TUAC_6[m,n])$ can be divided in three partitions
$E_6 = \{u,v \in V(TUAC_6[m,n]) | d_u = d_v = 3\}$,
$E_5 = \{u,v \in V(TUAC_6[m,n]) | d_u = 3, \textit{ and } d_v = 2\}$, and
$E_4 = \{u,v \in V(TUAC_6[m,n]) | d_u = d_v = 2\}$.

From Fig. 2, it is easy to see that the size of edge/bond partitions E_4, E_5 and E_6 are equal to are equal to m, $2m$ and $3mn - m$, respectively. From Fig. 3, one can see that for every atom/vertex $v \in V_2$, $S_v = 2+3 = 5$, since for its adjacent vertices u, w; $d_u = 2 \textit{ and } d_w = 3$ ($u \in V_2$, $w \in V_3$) and obviously $S_u = 5$. Whereas $S_w = 2 \times 3 + 2$, since for $N(w) = \{u_1, u_2, v\}$, the degree of vertices/atoms u_1, u_2 equal to three. Also, for all other vertices a (which belong to V_3), $S_a = 3 \times 3 = 9$.

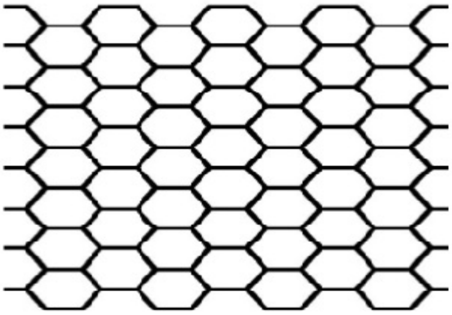

Figure 2. The 2D lattice of Armchair polyhex nanotubes $TUAC_6[m,n]$.

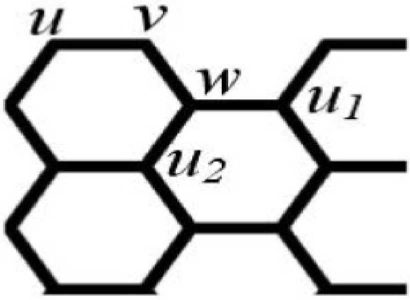

Figure 3. The particular of 2D lattice of Armchair polyhex $TUAC_6[m,n]$.

2.1 Arithmetic-Geometric (AG_2) Index

Let $G = (V,E)$ be a molecular graph, and $S_G(u)$ is the degree of the vertex u, then AG_2 index of G is defined as

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}},$$

where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

and

$$N_G(u) = \{v \in V(G)|uv \in E(G)\}.$$

2.2 SK_3 Index

The SK_3 index of a graph $G = (V,E)$ is defined as

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2},$$

where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

and

$$N_G(u) = \{v \in V(G) | uv \in E(G)\}.$$

2.3 Sanskruti Index

Recently, Hosamani [18], studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G.

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u) S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3,$$

where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

and

$$N_G(u) = \{v \in V(G) | uv \in E(G)\}.$$

3 Main Results

Table 1. Edge partition of graph of $TUAC6[m,n]$ armchair polyhex nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_u, S_v), where $u,v \in E(H)$	(5,5)	(5,8)	(8,8)	(8,9)	(9,9)
Number of edges	m	$2m$	m	$2m$	$9mn - 4m$

Theorem 3.1. *Let G be the armchair nanotube $TUAC_6[m,n]$ $\forall\ m,n \in E(G)$. Then the AG_2 index of G is equal to*

$$AG_2(G) = (9n - 2.0588)\, m.$$

Proof.

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}}.$$

This implies that

$$\begin{aligned}AG_2(TUAC_6[m,n]) &= (5,5)\left(\frac{5+5}{2\sqrt{25}}\right)+(5,8)\left(\frac{5+8}{2\sqrt{40}}\right)+(8,8)\left(\frac{8+8}{2\sqrt{64}}\right)\\&+(8,9)\left(\frac{8+9}{2\sqrt{72}}\right)+(9,9)\left(\frac{9+9}{2\sqrt{81}}\right)\\&= m\,(1)+(2m)\left(\frac{13}{2\sqrt{40}}\right)+(m)\,(1)+(2m)\left(\frac{17}{2\sqrt{72}}\right)+(9mn-4m)\,(1)\\&= 9mn-2m+\frac{13m}{\sqrt{40}}+\frac{17m}{\sqrt{72}}\\&= \left(9n-2+\frac{13}{\sqrt{40}}+\frac{17}{\sqrt{72}}\right)m\\&= (9n-2.0588)\,m.\end{aligned}$$

Theorem 3.2. *Let G be the armchair nanotube* $TUAC_6[m,n]$ $\forall\ m,n \in E(G)$. *Then the* SK_3 *index of G is equal to*

$$SK_3(G) = (81n+7)\,m.$$

Proof.

$$SK_3(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2}.$$

This implies that

$$\begin{aligned}SK_3(TUAC_6[m,n]) &= (5,5)\left(\frac{5+5}{2}\right)+(5,8)\left(\frac{5+8}{2}\right)+(8,8)\left(\frac{8+8}{2}\right)\\&+(8,9)\left(\frac{8+9}{2}\right)+(9,9)\left(\frac{9+9}{2}\right)\\&= m\,(5)+(2m)\left(\frac{13}{2}\right)+(m)\,(8)+(2m)\left(\frac{17}{2}\right)+(9mn-4m)\,(9)\\&= 5m+13m+8m+17m+81mn-36m\\&= 81mn+7m\\&= (81n+7)\,m.\end{aligned}$$

Theorem 3.3. *Let G be the armchair nanotube* $TUAC_6[m,n]$ $\forall\ m,n \in E(G)$. *Then the Sanskruti index of G is equal to*

$$S(G) = (1167.75n-75.58)\,m.$$

Proof.

$$S(G) = \sum_{uv\in E(G)} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2}\right)^3.$$

This implies that

$$\begin{aligned}
S(TUAC_6[m,n]) &= (5,5)\left(\frac{25}{5+5-2}\right)^3 + (5,8)\left(\frac{40}{5+8-2}\right)^3 + (8,8)\left(\frac{64}{8+8-2}\right)^3 \\
&+ (8,9)\left(\frac{72}{8+9-2}\right)^3 + (9,9)\left(\frac{81}{9+9-2}\right)^3 \\
&= m\left(\frac{25}{8}\right)^3 + 2m\left(\frac{40}{11}\right)^3 + m\left(\frac{64}{14}\right)^3 + 2m\left(\frac{72}{15}\right)^3 \\
&+ (9mn-4m)\left(\frac{81}{16}\right)^3 \\
&= m\,(3.125)^3 + 2m\,(3.6363)^3 + m\,(4.5714)^3 + 2m\,(4.8)^3 \\
&+ (9mn-4m)\,(5.0625)^3 \\
&= (1167.75n - 75.58)\,m.
\end{aligned}$$

Conclusion

In this paper, we have computed the value of AG_2 index, SK_3 index and Sanskruti index for $TUAC_6[m,n]$ armchair polyhex nanotube without using computer.

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Eng. Appl. Sci. Lett., Vol. **1***(2018), No. 1, pp. 01 - 09*
Website: https://pisrt.org/psr-press/journals/easl/
ISSN: 2617-9709 (Online) 2617-9695 (Print)
http://dx.doi.org/10.30538/psrp-easl2018.0001

SOME NUMERICAL INVARIANTS ASSOCIATED WITH V-PHENYLENIC NANOTUBE AND NANOTORI

RACHANNA KANABUR[1], SUNILKUMAR HOSAMANI

Abstract. A carbon nanotube (CNT) is a miniature cylindrical carbon structure that has hexagonal graphite molecules attached at the edges. In this paper, we compute the numerical invariant (Topological indices) of linear [n]-phenylenic, lattice of $C_4C_6C_8[m,n]$, $TUC_4C_6C_8[m,n]$ nanotube, $C_4C_6C_8[m,n]$ nanotori.

Index Terms: Molecular graph; topological index; nanotube; nanotori.

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [1, 2]. This theory had an important effect on the development of the chemical sciences. In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [2]. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [3].

Received 28-08-2018. Revised 01-09-2018. Accepted 20-09-2018.

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2. Computing the Topological Indices of Certain Nanotubes

In [4, 5, 6], Shigehalli and Kanabur have put forward new degree based topological indices viz. arithmetic-geometric index, SK index, SK_1 index and SK_2 index. Which are defined as follows: Let $G = (V, E)$ be a molecular graph,$d_G(u)$ and , $d_G(v)$ is the degree of the vertex u and v, then

$$AG_1 = \sum_{uv \in E(G)} \frac{1}{2\sqrt{d_u + d_v}}, \tag{1}$$

$$SK = \sum_{uv \in E(G)} \frac{d_u + d_v}{2}, \tag{2}$$

$$SK_1 = \sum_{uv \in E(G)} \frac{d_u d_v}{2}, \tag{3}$$

$$SK_2 = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2. \tag{4}$$

where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G. In this paper we give explicit formulae for these topological indices of [n]-phenylenic, lattice of $C_4C_6C_8[m, n]$, $TUC_4C_6C_8[m, n]$ nanotube, $C_4C_6C_8[m, n]$ nanotori [7, 8].

3. Main Results

The aim of this section, at first, is to compute some topological indices of the molecular graph of linear[n]-phenylenic as depicted in Fig.1

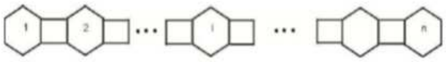

Figure 1. The molecular graph of a linear [n]-phenylenic.

It is easy to see that $T = T[n]$ has 6n vertices and $8n - 2$ edges, We partition the edges of T into three subsets $E_1(T)$, $E_2(T)$ and $E_3(T)$, Table1 shows the number of three types of edges.

Table 1. The number of three types of edges of the graph T.

(d_u, d_v)	Number of edges
(2,2)	6
(2,3)	$4n - 4$
(3,3)	$4n - 4$

From this table, we given an explicit computing formula for some indices of a linear [n]-phenylenic, as shown in above graph.

Theorem 3.1. *Consider the graph T of a linear[n]-phenylenic. Then the AG_1, SK, SK_1 and SK_2 indices of T are equal to*

(1) $AG_1(G) = 8.08n - 2.08$,
(2) $SK(G) = 22n - 10$,
(3) $SK_1(G) = 30n - 18$,
(4) $SK_2(G) = 61n - 37$.

Proof. (1)

$$\begin{aligned}
AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\
&= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\
&\quad + \sum_{uv\in E_3(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\
&= |E_1(G)|\frac{2+2}{2\sqrt{2.2}} + |E_2(G)|\frac{2+3}{2\sqrt{2.3}} \\
&\quad +|E_3(G)|\frac{3+3}{2\sqrt{3.3}} \\
&= 6(1) + (4n-4)\left(\frac{5}{2\sqrt{6}}\right) + (4n-4)(1) \\
&= 8.08n - 2.08.
\end{aligned}$$

(2)

$$\begin{aligned}
SK(G) &= \sum_{uv\in E(G)} \frac{d_u+d_v}{2} \\
&= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2} \\
&\quad + \sum_{uv\in E_3(G)} \frac{d_u+d_v}{2} \\
&= |E_1(G)|\frac{2+2}{2} + |E_2(G)|\frac{2+3}{2} \\
&\quad +|E_3(G)|\frac{3+3}{2} \\
&= 12 + 10n - 10 + 12n - 12 \\
&= 22n - 10.
\end{aligned}$$

(3)

$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{2}$$

$$\begin{aligned}
&= \sum_{uv\in E_1(G)} \frac{d_u d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u d_v}{2} \\
&\quad + \sum_{uv\in E_3(G)} \frac{d_u d_v}{2} \\
&= |E_1(G)|\frac{2.2}{2} + |E_2(G)|\frac{2.3}{2} \\
&\quad +|E_3(G)|\frac{3.3}{2} \\
&= = 12 + 12n - 12 + 18n - 18 \\
&= 30n - 18.
\end{aligned}$$

(4)

$$\begin{aligned}
SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&= \sum_{uv\in E_1(G)} \left(\frac{d_u + d_v}{2}\right)^2 + \sum_{uv\in E_2(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&\quad + \sum_{uv\in E_3(G)} \left(\frac{d_u + d_v}{2}\right)^2 \\
&= |E_1(G)| \left(\frac{2+2}{2}\right)^2 + |E_2(G)| \left(\frac{2+3}{2}\right)^2 \\
&\quad +|E_3(G)| \left(\frac{3+3}{2}\right)^2 \\
&= 24 + 25n - 25 + 36n - 36 \\
&= 61n - 37.
\end{aligned}$$

□

In continue of this section, we see the following figures

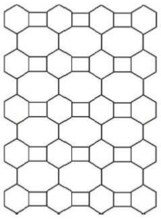

Figure 2. The 2-D graph lattice of $C_4C_6C_8[4,5]$ nanotube.

We now consider the molecular graph $G = C_4C_6C_8[m,n]$, Fig.2. It is easy to see that $|V(G)| = 6mn$ and $|E(G)| = 9mn - 2n - m$, We partition the edges of

G into three subsets $E_1(G)$, $E_2(G)$ and $E_3(G)$. The number of three types of edges is shown in Table 2.

TABLE 2. The number of three types of edges of the graph T.

(d_u, d_v)	Number of edges
(2,2)	$2n+4$
(2,3)	$4m+4n-8$
(3,3)	$9mn-8n-5m+4$

From this table, we have given an explicit computing of some indices of G (Fig. 2).

Theorem 3.2. *Consider the graph T of a linear[n]-phenylenic. Then the AG_1, SK, SK_1 and SK_2 indices of T are equal to*

(1) $AG_1(G) = (9n - 5.92)m - 9.92n - 3.84$,
(2) $SK(G) = (27n - 5)m - 10n$,
(3) $SK_1(G) = (40.5n - 10)m - 20n + 2$,
(4) $SK_2(G) = (81n - 20)m - 39n - 48$.

Proof. (1)

$$\begin{aligned} AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\ &= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\ &\quad + \sum_{uv\in E_3(G)} \frac{d_u+d_v}{2\sqrt{d_u.d_v}} \\ &= |E_1(G)|\frac{2+2}{2\sqrt{2.2}} + |E_2(G)|\frac{2+3}{2\sqrt{2.3}} \\ &\quad +|E_3(G)|\frac{3+3}{2\sqrt{3.3}} \\ &= 9mn - 5.92m - 9.92n - 3.04 \\ &= = (9n - 5.92)m - 9.92n - 3.84. \end{aligned}$$

(2)

$$\begin{aligned} SK(G) &= \sum_{uv\in E(G)} \frac{d_u+d_v}{2} \\ &= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2} \\ &\quad + \sum_{uv\in E_3(G)} \frac{d_u+d_v}{2} \end{aligned}$$

$$\begin{aligned} &= |E_1(G)|\frac{2+2}{2}+|E_2(G)|\frac{2+3}{2} \\ &\quad +|E_3(G)|\frac{3+3}{2} \\ &= = 4n+8+10m+10n-20+27mn-24n-15m+12 \\ &= 27mn-10n-5m. \end{aligned}$$

(3)

$$\begin{aligned} SK_1(G) &= \sum_{uv\in E(G)} \frac{d_u d_v}{2} \\ &= \sum_{uv\in E_1(G)} \frac{d_u d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u d_v}{2} \\ &\quad + \sum_{uv\in E_3(G)} \frac{d_u d_v}{2} \\ &= |E_1(G)|\frac{2.2}{2}+|E_2(G)|\frac{2.3}{2} \\ &\quad +|E_3(G)|\frac{3.3}{2} \\ &= = 4n+8+12m+12n-24+40.5mn-36n-22.5m+8 \\ &= (40.5n-10)m-20n+2. \end{aligned}$$

(4)

$$\begin{aligned} SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\ &= \sum_{uv\in E_1(G)} \left(\frac{d_u+d_v}{2}\right)^2 + \sum_{uv\in E_2(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\ &\quad + \sum_{uv\in E_3(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\ &= |E_1(G)|\left(\frac{2+2}{2}\right)^2+|E_2(G)|\left(\frac{2+3}{2}\right)^2 \\ &\quad +|E_3(G)|\left(\frac{3+3}{2}\right)^2 \\ &= 8n+16+25m+25n-100+81mn-72n-45m+36 \\ &= (81n-20)m-39n-48. \end{aligned}$$

□

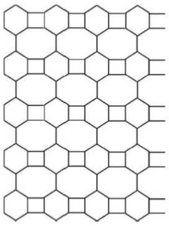

Figure 3. The 2-D graph lattice of $TUC_4C_6C_8[4,5]$ nanotube.

We now consider the molecular graph $K = TUC_4C_6C_8[m,n]$, Fig. 3. It is easy to see that $|V(K)| = 6mn$ and $|E(K)| = 9mn - n$. We partition the edges of nanotube K into two subsets $E_1(G)$, $E_2(G)$ and compute the total number of edges for the 2-dimensional of graph K (Table 3).

Table 3. The number of three types of edges of the graph T.

(d_u, d_v)	Number of edges
(2,3)	$4n$
(3,3)	$9mn - 5m$

From this table, we given an explicit computing formula for some indices of a linear [n]-phenylenic, as shown in above graph.

Theorem 3.3. *Consider the graph T of a linear[n]-phenylenic. Then the AG_1, SK, SK_1 and SK_2 indices of T are equal to*

1. $AG_1(G) = (9n - 0.92)m,$
2. $SK(G) = (27n - 5)m.,$
3. $SK_1(G) = (40.5n - 10.5)m.,$
4. $SK_2(G) = (81n - 20)m..$

Proof. (1)

$$\begin{aligned}
AG_1(G) &= \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\
&= \sum_{uv\in E_1(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} + \sum_{uv\in E_2(G)} \frac{d_u + d_v}{2\sqrt{d_u.d_v}} \\
&= |E_1(G)|\frac{2+3}{2\sqrt{2.2}} + |E_2(G)|\frac{3+3}{2\sqrt{2.3}} \\
&= 9mn - 5m + 4.08m \\
&= (9n - 0.92)m.
\end{aligned}$$

(2)

$$SK(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2}$$

$$\begin{aligned} &= \sum_{uv\in E_1(G)} \frac{d_u+d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u+d_v}{2} \\ &= |E_1(G)|\frac{2+3}{2} + |E_2(G)|\frac{3+3}{2} \\ &= 10m + 27mn - 15m \\ &= (27n-5)m. \end{aligned}$$

(3)

$$\begin{aligned} SK_1(G) &= \sum_{uv\in E(G)} \frac{d_u d_v}{2} \\ &= \sum_{uv\in E_1(G)} \frac{d_u d_v}{2} + \sum_{uv\in E_2(G)} \frac{d_u d_v}{2} \\ &= |E_1(G)|\frac{2.3}{2} + |E_2(G)|\frac{3.3}{2} \\ &= = 12mn + (9mn - 5m)(4.5) \\ &= (40.5n - 10.5)m. \end{aligned}$$

(4)

$$\begin{aligned} SK_2(G) &= \sum_{uv\in E(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\ &= \sum_{uv\in E_1(G)} \left(\frac{d_u+d_v}{2}\right)^2 + \sum_{uv\in E_2(G)} \left(\frac{d_u+d_v}{2}\right)^2 \\ &= |E_1(G)|\left(\frac{2+3}{2}\right)^2 + |E_2(G)|\left(\frac{3+3}{2}\right)^2 \\ &= 25m + 81mn - 45m \\ &= (81n-20)m. \end{aligned}$$

□

4. conclusion

In this paper, we have computed the value of AG_1 index, SK index, SK_1 index and SK_2 index for Linear [n]-phenylenic, lattice of $C_4C_6C_8[m,n]$, $TUC_4C_6C_8[m,n]$ nanotube, $C_4C_6C_8[m,n]$ nanotori without using computer.

Competing Interests

The authors declare that they have no competing interests.

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Article *in* Journal of Computer and Mathematical Sciences · October 2018

DOI: 10.29055/jcms/886

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Journal of Computer and Mathematical Sciences, *Vol.9(10),1440-1453 October 2018* *ISSN 0976-5727 (Print)*
(An International Research Journal), *www.compmath-journal.org* *ISSN 2319-8133 (Online)*

Study of Degree-Based Topological Indices of Some Nanotubes

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(Received on: September 26, 2018)

ABSTRACT

Recently[10], Shigehalli and Kanabur have introduced two new topological indices namely, AG_2 index and SK_3 index. Hosamani[13], has studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G. In this paper, formula for computing the some nanotube family is given.

Keywords: Molecular graph, Arithmetic-Geometric index (AG_2 index), SK_3 index, Sanskruti index and some nanotubes.

1. INTRODUCTION

Let G be a simple connected graph in chemical graph theory. In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted[1].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena[1,2]. This theory had an important effect on the development of the chemical sciences.

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G=(V,E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by du and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv[1].

2. COMPUTING DEGREE-BASED TOPOLOGICAL INDICES

In[9, 10,11 and 13], Shigehalli and Kanabur have put forward new degree based topological indices viz. arithmetic-geometric index, SK index, SK_1 index, SK_2 index, SK_3 index, AG_2 index and Sanskruti index Which are defined as follows:

Let $G = (V, E)$ be a molecular graph, and $d_G(u)$, $d_G(v)$ is the degree of the vertex u *and* v, and $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$S_G(u) = \sum_{u,v\in E(G)} d_G(u)$ and $N_G(u) = \{v \in V(G)/uv \in E(G)\}$

$$AG_1(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}} \tag{1}$$

$$SK(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2} \tag{2}$$

$$SK_1(G) = \sum_{u,v\in E(G)} \frac{d_G(u).d_G(v)}{2} \tag{3}$$

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2 \tag{4}$$

$$SK_3(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2} \tag{5}$$

$$AG_2(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u).S_G(v)}} \tag{6}$$

$$S(G) = \sum_{uv\in E(G)} \left(\frac{S_G(u)\,S_G(v)}{S_G(u)+S_G(v)-2}\right)^3 \tag{7}$$

3.1. Computing Degree-Based Topological Indices of Certain Nanostructures

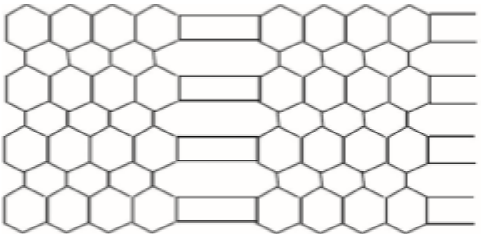

Figure 3.1

The above figure3.4 by algebraic method, we get $\left|V \;\; G\right| = 18pq$ & $\left|E \;\; F\right| = 27pq - 4p.$ Further .the edge degree partition of is given in below table3.1.

Table3.1: The edge degree partition of the nanostructure G=G [p,q]

$d_G(e),d_G(f)\backslash e\text{-}f \in E(G)$	(2,2)	(3,2)	(3,3)
Number of edges	0	16p	27pq-20p

Theorem3.1.1: Let *G= (V, E)* be the graph of G=G [p,q]. Then the AG_1 index of *G* are given as

$$AG_1\,(G) = 27pq-3.67006p$$

Proof: To compute the $AG_1\,(G)$ index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$\text{AG}_1\text{ (G)} = \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2\sqrt{d_G(e).d_G(f)}}\right]$$

$$\text{AG}_1\text{ (G)} = (2,2)\left[\frac{2+2}{2\sqrt{2(2)}}\right]+(3,2)\left[\frac{3+2}{2\sqrt{3(2)}}\right]+(3,3)\left[\frac{3+3}{2\sqrt{3(3)}}\right]$$

$$= 0(1)+16p\left(\frac{5}{2\sqrt{6}}\right)+(27pq-20p)(1)$$

$$= 0+16.32993p+27pq-20p$$

$$= 27pq-3.67006p$$

Theorem3.1.2: Let *G= (V, E)* be the graph of G=G [p,q]. Then the *SK* index of *G* are given as

$$SK(G) = 81pq-20p$$

Proof: To compute the *SK (G)* index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$\text{SK(G)} = \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2}\right]$$

$$\text{SK(G)} = (2,2)\left[\frac{2+2}{2}\right]+(3,2)\left[\frac{3+2}{2}\right]+(3,3)\left[\frac{3+3}{2}\right]$$

$$= (0)(2)+16P\left(\frac{5}{2}\right)+(27pq-20p)(3)$$

$$= 0+40p+81pq-60p$$

$$= 81pq-20p$$

Theorem3.1.3: Let *G= (V, E)* be the graph of G=G [p,q]. Then the SK_1 index of *G* are given as

$$SK_1(G) = 121.5pq-42p$$

Proof: To compute the $SK_1(G)$ index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$SK_1(G) = \sum_{e,f\in E(G)}\left[\frac{d_G(e).d_G(f)}{2}\right]$$

$$SK_1(G) = (2,2)\left[\frac{2(2)}{2}\right]+(3,2)\left[\frac{3(2)}{2}\right]+(3,3)\left[\frac{3(3)}{2}\right]$$

$$= 0(2)+16p(3)+(27pq-20p)\left(\frac{9}{2}\right)$$

$$= 0+48p+121.5pq-90p$$

$$= 121.5pq-42p$$

Theorem3.1.4: Let *G= (V, E)* be the graph of G=G [p,q]. Then the SK_2 index of *G* are given as

$$SK_2(G) = 81pq-80p$$

Proof: To compute the $SK_2(G)$ index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$SK_2(G) = \sum_{e,f\in E(G)}\left[\frac{d_G(e)+d_G(f)}{2}\right]^2$$

$$SK_2(G) = (2,2)\left[\frac{2+2}{2}\right]^2+(3,2)\left[\frac{3+2}{2}\right]^2+(3,3)\left[\frac{3+3}{2}\right]^2$$

$$= 0(2)^2+16p(2.5)^2+(27pq-20p)\ 9$$

$$= 0+100p+81pq-180p$$

$$= 81pq-80p$$

3.2. Computing Degree-Based Topological Indices of $TURC_4C_8(8)$ Nanotubes

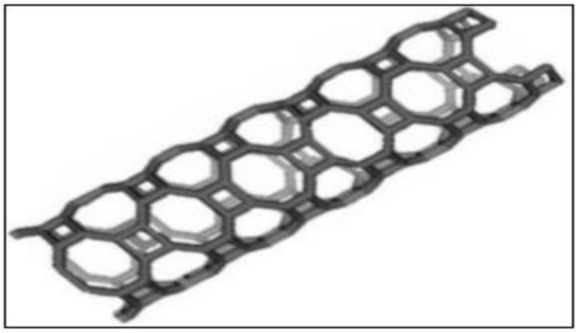

Figure 3.2

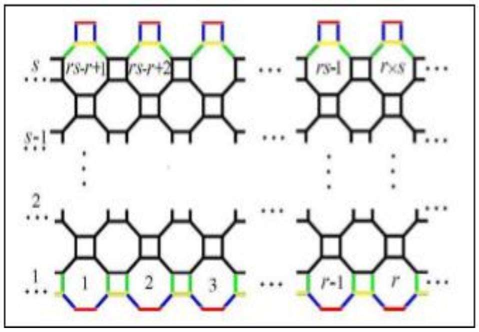

Figure 3.3

Table3.2: Summation of degrees of end points.

Summation of degrees of edge end point	$e_{(5,5)}$	$e_{(5,8)}$	$e_{(8,8)}$	$e_{(8,9)}$	$e_{(9,9)}$
Number of edges of this type	2r	4r	2r	4r	12r-11r

Theorem3.2.1: Let $G= (V, E)$ be the graph of $TURC_4C_8$ (8). Then the AG_2 index of G are given as

$$AG_2\ (G) = \quad 16.1176r$$

Proof: To compute the $AG_2\ (G)$ index of the $TURC_4C_8$ (8).

$$AG_2(G)= \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2\sqrt{S_G\ \ u\ \ S_G\ \ v}} \right]$$

$$=e_{(5,5)} \left[\frac{5+5}{2\sqrt{5(5)}} \right] +e_{(5,8)} \left[\frac{5+8}{2\sqrt{5(8)}} \right] +e_{(8,8)} \left[\frac{8+8}{2\sqrt{8(8)}} \right] +e_{(8,9)} \left[\frac{8+9}{2\sqrt{8(9)}} \right]$$

$$+e_{(9,9)} \left[\frac{9+9}{2\sqrt{9(9)}} \right]$$

$$=2r \left[\frac{25}{2(5)} \right] +4r \left[\frac{13}{2\sqrt{40}} \right] +2r \left[\frac{16}{2(8)} \right] +4r \left[\frac{17}{2\sqrt{72}} \right] +(12r\text{-}11r) \left[\frac{18}{2(9)} \right]$$

=2r(2.5)+4r(1.0277)+2r(1)+4r(1.0017)+(12r-11r) (1)
=16.1176r

Theorem3.2.2: Let $G= (V, E)$ be the graph of $TURC_4C_8$ (8). Then the SK_3 index of G are given as

$$SK_3\ (G) = 95r$$

Proof: To compute the $SK_3\ (G)$ index of the $TURC_4C_8$ (8).

$$SK_3= \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2} \right]$$

$$=e_{(5,5)} \left[\frac{5+5}{2} \right] +e_{(5,8)} \left[\frac{5+8}{2} \right] +e_{(8,8)} \left[\frac{8+8}{2} \right] +e_{(8,9)} \left[\frac{8+9}{2} \right] +e_{(9,9)} \left[\frac{9+9}{2} \right]$$

=2r(5)+4r(6.5)+2r(8)+4r(8.5)+(12r-11r) (9)
= 95r

Theorem3.2.3: Let $G= (V, E)$ be the graph of $TURC_4C_8$ (8). Then the Sanskruti index of G are given as

$$S\ (G) =1016.5527r$$

Proof: To compute the Sanskruti index of the $TURC_4C_8$ (8).

$$S(G)=\sum_{u,v\in E(G)}\left[\frac{S_G\ \ u\ \ .S_G\ \ v}{S_G\ \ u\ \ +S_G\ \ v\ \ -2}\right]^3$$

$$= e_{(5,5)}\left[\frac{5(5)}{5+5-2}\right]^3 +e_{(5,8)}\left[\frac{5(8)}{5+8-2}\right]^3 +e_{(8,8)}\left[\frac{8(8)}{8+8-2}\right]^3$$

$$+ e_{(8,9)}\left[\frac{8(9)}{8+9-2}\right]^3 +e_{(9,9)}\left[\frac{9(9)}{9+9-2}\right]^3$$

$$= 2r\left[\frac{25}{8}\right]^3 +4r\left[\frac{40}{11}\right]^3 +2r\left[\frac{64}{14}\right]^3 +4r\left[\frac{72}{15}\right]^3 +(12r-11r)\left[\frac{81}{16}\right]^3$$

$$=2r(30.5175)+4r(48.0841)+2r(95.5335)+4r(110.592)+ (12r-11r)\ (129.7463)$$

$$=1016.5527$$

3.3. Computing Degree-Based Topological Indices of Sierpinski Networks.

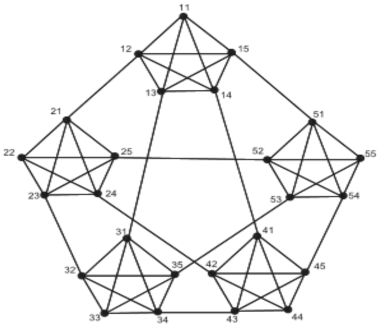

Figure 3.4

Table3.3: Edge partition of S(n,k) sierpinski network based on degrees of end vertices of each edge.

(d_u,d_v) where $u,v\in E(G)$	(k-1,k)	(k,k)
Number of edges	2k	$\dfrac{k^{n+1}-5k}{2}$

Theorem3.3.1: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the AG_1 index of *G* are given as

$$AG_1\ (G) = \left[\frac{2k^2-k}{\sqrt{k^2-k}}\right]+\left[\frac{k^{n+1}-5k}{2}\right]$$

Proof: To compute the $AG_1\ (G)$ index of the Sierpinski Networks.

$$AG_1(G) = \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2\sqrt{d_G(e).d_G(f)}}\right]$$

$$=(k-1,k)\left[\frac{(k-1)+k}{2\sqrt{(k-1)k}}\right]+(k,k)\left[\frac{k+k}{2\sqrt{(k)k}}\right]$$

$$=2k\left[\frac{2k-1}{2\sqrt{k^2-k}}\right]+\left[\frac{k^{n+1}-5k}{2}\right]\left[\frac{2k}{2\sqrt{k^2}}\right]$$

$$=\left[\frac{k(2k-1)}{\sqrt{k^2-k}}\right]+\frac{k^{n+1}-5k}{2}(1)$$

$$=\left[\frac{2k^2-k}{\sqrt{k^2-k}}\right]+\left[\frac{k^{n+1}-5k}{2}\right]$$

Theorem3.3.2: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the *SK* index of *G* are given as

$$SK(G) = 4.5k^2-k+\left[\frac{k^{n+2}}{2}\right]$$

Proof: To compute the *SK (G)* index of the Sierpinski Networks.

$$SK(G)= \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2}\right]$$

$$= (k-1,k)\left[\frac{k-1+k}{2}\right]+(k,k)\left[\frac{k+k}{2}\right]$$

$$= 2k\left[\frac{2k-1}{2}\right]+\left[\frac{k^{n+1}-5k}{2}\right]\left[\frac{k+k}{2}\right]$$

$$= k(2k-1)+\left[\frac{k^{n+1}-5k}{2}\right]k$$

$$= (2k^2-k)+\left[\frac{k^{n+2}-5k^2}{2}\right]$$

$$= 4.5k^2-k+\left[\frac{k^{n+2}}{2}\right]$$

Theorem3.3.3: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the SK_1 index of *G* are given as

$$SK_1\,(G) = \frac{k^{n+3}-k^3-4k}{4}$$

Proof: To compute the $SK_1\,(G)$ index of the Sierpinski Networks.

$$\mathrm{SK}_1(\mathrm{G}) = \sum_{e,f\in E(G)}\left[\frac{d_G(e).d_G(f)}{2}\right]$$

$$= (\mathrm{k}\text{-}1,\mathrm{k})\left[\frac{(k-1)k}{2}\right]+(\mathrm{k},\mathrm{k})\left[\frac{(k)k}{2}\right]$$

$$= 2\mathrm{k}\left[\frac{k^2-k}{2}\right]+\left[\frac{k^{n+1}-5k}{2}\right]\left[\frac{k^2}{2}\right]$$

$$= (\mathrm{k}^3\text{-}\mathrm{k})+\left[\frac{k^{n+3}-5k^3}{4}\right]$$

$$= \frac{k^{n+3}-k^3-4k}{4}$$

Theorem3.3.4: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the SK_2 index of *G* are given as

$$SK_2\,(G) = \frac{k^{n+3}-k^3-4k^2+k}{8}$$

Proof: To compute the $SK_2\,(G)$ index of the Sierpinski Networks.

$$\mathrm{SK}_2(\mathrm{G}) = \sum_{e,f\in E(G)}\left[\frac{d_G(e)+d_G(f)}{2}\right]^2$$

$$= (\mathrm{k}\text{-}1,\mathrm{k})\left[\frac{(k-1)+k)}{2}\right]^2+(\mathrm{k},\mathrm{k})\left[\frac{k+k}{2}\right]^2$$

$$= 2\mathrm{k}\left[\frac{4k^2+1-4k}{2}\right]^2+\left[\frac{k^{n+1}-5k}{2}\right]\mathrm{k}^2$$

$$= \left[\frac{4k^3+k-4k^2}{2}\right]+\left[\frac{k^{n+3}-5k^3}{8}\right]$$

$$= \frac{k^{n+3}-k^3-4k^2+k}{8}$$

Table3.4: Edge partition of graph S(n,k) where n=2 based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_u,S_v) where $u,v \in E(G)$	(k^2-k,k^2-1)	(k^2-1,k^2-1)
Number of edges	k^2-k	$\frac{k(k^n-2k+1)}{2}$

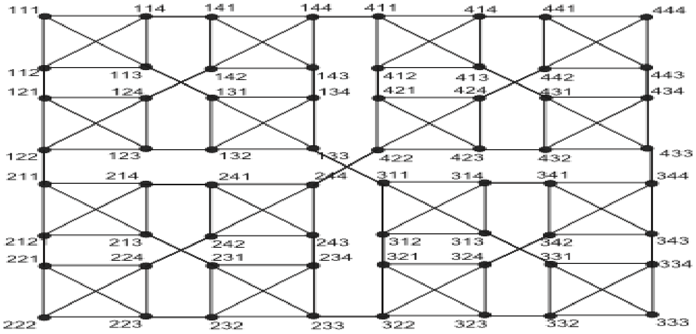

Figure 3.5

Theorem3.3.5: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the AG_2 index of *G* are given as

$$AG_2\,(G) = \left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k^{n+1}-2k^2+k}{2}\right]$$

Proof: To compute the $AG_2\,(G)$ index of the Sierpinski Networks.

$$AG_2\,(G) = \sum_{u,v\in E(G)}\left[\frac{Su+Sv}{2\sqrt{Su(Sv)}}\right]$$

$$= (k^2-k,k^2-1)\left[\frac{k^2-k+k^2-1}{2\sqrt{(k^2-k)(k^2-1)}}\right]+(k^2-1,k^2-1)\left[\frac{k^2-1+k^2-1}{2\sqrt{(k^2-1)(k^2-1)}}\right]$$

$$= (k^2-k)\left[\frac{2k^2-k-1}{2\sqrt{k^4-k^2-k^3+k}}\right]+\left[\frac{k(k^n-2k+1)}{2}\right]\left[\frac{2k^2-2}{2(k^2-1)}\right]$$

$$=\left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k^{n+1}-2k^2+k}{2}\right]$$

Theorem3.3.6: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the SK_3 index of *G* are given as

$$SK_3\,(G) = \left[\frac{2k^{n+3} - 2k^{n+1} + 2k^4 - 4k^3 + 4k^2}{4}\right]$$

Proof: To compute the $SK_3\,(G)$ index of the Sierpinski Networks.

$$\mathrm{SK}_3\,(\mathrm{G}) = \sum_{u,v \in E(G)} \left[\frac{S_G\ \ u\ + S_G\ \ v}{2}\right]$$

$$=(k^2-k,k^2-1)\left[\frac{k^2 - k + k^2 - 1}{2}\right] + (k^2-1,k^2-1)\left[\frac{k^2 - 1 + k^2 - 1}{2}\right]$$

$$= (k^2-k)\left[\frac{2k^2 - k - 1}{2}\right] + \left[\frac{k(k^n - 2k + 1)}{2}\right]\left[\frac{2k^2 - 2}{2}\right]$$

$$= \left[\frac{2k^4 - 3k^3 + k}{2}\right] + \left[\frac{(2k^2 - 2)(k^{n+1} - 2k^2 + k}{4}\right]$$

$$= \left[\frac{4k^4 - 6k^3 + 2k + 2k^{n+3} - 2k^4 + 2k^3 - 2k^{n+1} + 4k^2 - 2k}{4}\right]$$

$$= \left[\frac{2k^{n+3} - 2k^{n+1} + 2k^4 - 4k^3 + 4k^2}{4}\right]$$

Theorem3.3.37: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the Sanskruti index of *G* are given as

$$S\,(G) = (k^2-k)\left[\frac{k^4 - k^3 - k^2 + k}{2k^2 - k - 3}\right]^3 + \left[\frac{k(k^n - 2k + 1)}{2}\right]\left[\frac{k^4 - 2k^2 + 1}{2k^2 - 4}\right]^3$$

Proof: To compute the Sanskruti index of the Sierpinski Networks.

$$\mathrm{S(G)} = \sum_{u,v \in E(G)} \left[\frac{S_G\ \ u\ .S_G\ \ v}{S_G\ \ u\ + S_G\ \ v\ - 2}\right]^3$$

$$= (k^2-k,k^2-1)\left[\frac{(k^2 - k)(k^2 - 1)}{k^2 - k + k^2 - 1 - 2}\right]^3 + (k^2-1,k^2-1)\left[\frac{(k^2 - 1)(k^2 - 1)}{k^2 - 1 + k^2 - 1 - 2}\right]^3$$

$$= (k^2-k)\left[\frac{k^4 - k^3 - k^2 + k}{2k^2 - k - 3}\right]^3 + \left[\frac{k(k^n - 2k + 1)}{2}\right]\left[\frac{k^4 - 2k^2 + 1}{2k^2 - 4}\right]^3$$

Table3.5: n$\geq$3

(S_u,S_v) where u,v$\in$E(G)	(k^2-k,k^2-1)	(k^2-1,k^2-1)	(k^2-1,k^2)	(k^2,k^2)
Number of edges	k^2-k	$\frac{k(k^n-3k+2)}{2}$	k^2-k	$\frac{k(k^n-k^2-k+1)}{2}$

Theorem3.3.8: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the AG_2 index of *G* are given as

$$AG_2\,(G) = \left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right] + \left[\frac{2k^4-3k^2+k}{2\sqrt{k^4-k^2}}\right] + \left[\frac{k^{n+1}-4k^2+2k-1}{2}\right]$$

Proof: To compute the $AG_2\,(G)$ index of the Sierpinski Networks.

$$\text{AG}_2\text{(G)=} \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2\sqrt{S_G\ \ u\ \ S_G\ \ v}}\right]$$

$$=(k^2\text{-}k,k^2\text{-}1)\left[\frac{k^2-k+k^2-1}{2\sqrt{(k^2-k)(k^2-1)}}\right]+(k^2\text{-}1,k^2\text{-}1)\left[\frac{k^2-1+k^2-1}{2\sqrt{(k^2-1)(k^2-1)}}\right]$$

$$+(k^2\text{-}1,k^2)\left[\frac{k^2-1+k^2}{2\sqrt{(k^2-1)k^2}}\right]+(k^2,k^2)\left[\frac{k^2+k^2}{2\sqrt{k^2(k^2)}}\right]$$

$$=(k^2\text{-}k)\left[\frac{2k^2-k-1}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k(k^2-3k+2)}{2}\right]\left[\frac{2k^2-2}{2(k^2-1)}\right]$$

$$+(k^2\text{-}k)\left[\frac{2k^2-1}{2\sqrt{k^4-k^2}}\right]+\left[\frac{k(k^n-k^2-k+1}{2}\right]\left[\frac{2k^2}{2k^2}\right]$$

$$=\left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k^3-3k^2+2k}{2}\right]+\left[\frac{2k^4-3k^2+k}{2\sqrt{k^4-k^2}}\right]+$$

$$\left[\frac{k^{n+1}-k^3-k^2+1}{2}\right]$$

$$=\left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{2k^4-3k^2+k}{2\sqrt{k^4-k^2}}\right]+\left[\frac{k^{n+1}-4k^2+2k-1}{2}\right]$$

Theorem3.3.9: Let *G= (V, E)* be the graph of Sierpinski Networks .Then the SK_3 index of *G* are given as

$$SK_3\,(G) = \left[\frac{k^{n+3}-3k^3+2k^2}{2}\right]$$

Proof: To compute the *SK_3 (G)* index of the Sierpinski Networks.

$$\mathrm{SK}_3 = \sum_{u,v\in E(G)}\left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2}\right]$$

$$= (k^2\text{-}k,k^2\text{-}1)\left[\frac{k^2-k+k^2-1}{2}\right]+(k^2\text{-}1,k^2\text{-}1)\left[\frac{k^2-1+k^2-1}{2}\right]$$

$$+(k^2\text{-}1,k^2)\left[\frac{k^2-1+k^2}{2}\right]+(k^2,k^2)\left[\frac{k^2+k^2}{2}\right]$$

$$=(k^2\text{-}k)\left[\frac{2k^2-k-1}{2}\right]+\left[\frac{k(k^2-3k+2}{2}\right]\left[\frac{2k^2-2}{2}\right]+(k^2\text{-}k)\left[\frac{2k^2-1}{2}\right]$$

$$+\left[\frac{k(k^n-k^2-k+1}{2}\right]\left[\frac{2k^2}{2}\right]$$

$$=\left[\frac{2k^4-3k^3+k}{2}\right]+\left[\frac{(k^2-1)(k^3-3k^2+2k}{2}\right]+\left[\frac{2k^4-2k^3-k^2-k}{2}\right]$$

$$+\left[\frac{k^2(k^{n+1}-k^3-k^2+k)}{2}\right]$$

$$=\left[\frac{2k^4-3k^3+k+k^5-3k^4+2k^3-k^3+3k^2-2k+2k^4-2k^3-k^2-k+k^{n+3}-k^5-k^4+k^3}{2}\right]$$

$$=\left[\frac{k^{n+3}-3k^3+2k^2}{2}\right]$$

Theorem3.3.10: Let *G= (V, E)* be the graph of Sierpinski Networks .Then the Sanskruti index of *G* are given as

$$S\,(G) = (k^2\text{-}k)\left[\frac{k^4-k^3-k^2+k}{2k^2-k-3}\right]^3+\left[\frac{k(k^2-3k+2)}{2}\right]\left[\frac{k^4-2k^2+1}{2k^2-4}\right]^3+(k^2\text{-}k)\left[\frac{k^4-k^2}{2k^2-3}\right]^3$$

$$+\left[\frac{k(k^n-k^2-k+1}{2}\right]\left[\frac{k^4}{2k^2-2}\right]^3$$

Proof: To compute the Sanskruti index of the Sierpinski Networks.

$$\mathrm{S(G)} = \sum_{u,v\in E(G)} \left[\frac{S_G \;\; u \;\; S_G \;\; v}{S_G \;\; u \;\; + S_G \;\; v \;\; -2} \right]^3$$

$$= (k^2\text{-}k,k^2\text{-}1)\left[\frac{(k^2-k)(k^2-1)}{k^2-k+k^2-1-2} \right]^3 +(k^2\text{-}1,k^2\text{-}1)\left[\frac{(k^2-1)(k^2-1)}{k^2-1+k^2-1-2} \right]^3$$

$$+(k^2\text{-}1,k^2)\left[\frac{(k^2-1)k^2}{k^2-1+k^2-2} \right]^3 +(k^2,k^2)\left[\frac{k^2(k^2)}{k^2+k^2-2} \right]^3$$

$$= (k^2\text{-}k)\left[\frac{k^4-k^3-k^2+k}{2k^2-k-3} \right]^3 + \left[\frac{k(k^2-3k+2)}{2} \right]\left[\frac{k^4-2k^2+1}{2k^2-4} \right]^3$$

$$+ (k^2\text{-}k)\left[\frac{k^4-k^2}{2k^2-3} \right]^3 + \left[\frac{k(k^n-k^2-k+1}{2} \right]\left[\frac{k^4}{2k^2-2} \right]^3$$

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Article *in* Journal of Computer and Mathematical Sciences · October 2018

DOI: 10.29055/jcms/886

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Journal of Computer and Mathematical Sciences, *Vol.9(10),1440-1453 October 2018* *ISSN 0976-5727 (Print)*
(An International Research Journal), *www.compmath-journal.org* *ISSN 2319-8133 (Online)*

Study of Degree-Based Topological Indices of Some Nanotubes

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(Received on: September 26, 2018)

ABSTRACT

Recently[10], Shigehalli and Kanabur have introduced two new topological indices namely, AG_2 index and SK_3 index. Hosamani[13], has studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G. In this paper, formula for computing the some nanotube family is given.

Keywords: Molecular graph, Arithmetic-Geometric index (AG_2 index), SK_3 index, Sanskruti index and some nanotubes.

1. INTRODUCTION

Let G be a simple connected graph in chemical graph theory. In mathematics chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. And also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted[1].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena[1,2]. This theory had an important effect on the development of the chemical sciences.

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G=(V,E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by du and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv[1].

2. COMPUTING DEGREE-BASED TOPOLOGICAL INDICES

In[9, 10,11 and 13], Shigehalli and Kanabur have put forward new degree based topological indices viz. arithmetic-geometric index, SK index, SK_1 index, SK_2 index, SK_3 index, AG_2 index and Sanskruti index Which are defined as follows:

Let $G = (V, E)$ be a molecular graph, and $d_G(u)$, $d_G(v)$ is the degree of the vertex u *and* v, and $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v) in G.

$S_G(u) = \sum_{u,v \in E(G)} d_G(u)$ and $N_G(u) = \{v \in V(G)/uv \in E(G)\}$

$$AG_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) . d_G(v)}} \tag{1}$$

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2} \tag{2}$$

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) . d_G(v)}{2} \tag{3}$$

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2 \tag{4}$$

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2} \tag{5}$$

$$AG_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u) . S_G(v)}} \tag{6}$$

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u) S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3 \tag{7}$$

3.1. Computing Degree-Based Topological Indices of Certain Nanostructures

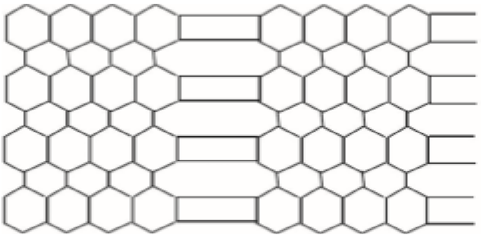

Figure 3.1

The above figure3.4 by algebraic method, we get $\left|V \ \ G\right| = 18pq$ & $\left|E \ \ F\right| = 27pq - 4p.$ Further .the edge degree partition of is given in below table3.1.

Table3.1: The edge degree partition of the nanostructure G=G [p,q]

$d_G(e),d_G(f)\backslash e\text{-}f \in E(G)$	(2,2)	(3,2)	(3,3)
Number of edges	0	16p	27pq-20p

Theorem3.1.1: Let *G= (V, E)* be the graph of G=G [p,q]. Then the AG_1 index of *G* are given as

$$AG_1\ (G) = 27pq-3.67006p$$

Proof: To compute the $AG_1\ (G)$ index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$\text{AG}_1\ (\text{G}) = \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2\sqrt{d_G(e).d_G(f)}} \right]$$

$$\text{AG}_1\ (\text{G}) = (2,2)\left[\frac{2+2}{2\sqrt{2(2)}}\right] + (3,2)\left[\frac{3+2}{2\sqrt{3(2)}}\right] + (3,3)\left[\frac{3+3}{2\sqrt{3(3)}}\right]$$

$$= 0(1)+16\text{p}\left(\frac{5}{2\sqrt{6}}\right)+(27\text{pq}-20\text{p})(1)$$

$$= 0+16.32993\text{p}+27\text{pq}-20\text{p}$$

$$= 27\text{pq}-3.67006\text{p}$$

Theorem3.1.2: Let *G= (V, E)* be the graph of G=G [p,q]. Then the *SK* index of *G* are given as

$$SK(G) = 81pq-20p$$

Proof: To compute the *SK (G)* index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$\text{SK(G)} = \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2} \right]$$

$$\text{SK(G)} = (2,2)\left[\frac{2+2}{2}\right] + (3,2)\left[\frac{3+2}{2}\right] + (3,3)\left[\frac{3+3}{2}\right]$$

$$= (0)(2)+16\text{P}\left(\frac{5}{2}\right)+(27\text{pq}-20\text{p})(3)$$

$$= 0+40\text{p}+81\text{pq}-60\text{p}$$

$$= 81\text{pq}-20\text{p}$$

Theorem3.1.3: Let *G= (V, E)* be the graph of G=G [p,q]. Then the SK_1 index of *G* are given as

$$SK_1(G) = 121.5pq-42p$$

Proof: To compute the $SK_1(G)$ index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$SK_1(G) = \sum_{e,f\in E(G)}\left[\frac{d_G(e).d_G(f)}{2}\right]$$

$$SK_1(G) = (2,2)\left[\frac{2(2)}{2}\right]+(3,2)\left[\frac{3(2)}{2}\right]+(3,3)\left[\frac{3(3)}{2}\right]$$

$$= 0(2)+16p(3)+(27pq-20p)\left(\frac{9}{2}\right)$$

$$= 0+48p+121.5pq-90p$$

$$= 121.5pq-42p$$

Theorem3.1.4: Let *G= (V, E)* be the graph of G=G [p,q]. Then the SK_2 index of *G* are given as

$$SK_2(G) = 81pq-80p$$

Proof: To compute the $SK_2(G)$ index of the G=G [p,q]. We need an edge partition of the G=G [p,q].

$$SK_2(G) = \sum_{e,f\in E(G)}\left[\frac{d_G(e)+d_G(f)}{2}\right]^2$$

$$SK_2(G) = (2,2)\left[\frac{2+2}{2}\right]^2+(3,2)\left[\frac{3+2}{2}\right]^2+(3,3)\left[\frac{3+3}{2}\right]^2$$

$$= 0(2)^2+16p(2.5)^2+(27pq-20p)\ 9$$

$$= 0+100p+81pq-180p$$

$$= 81pq-80p$$

3.2. Computing Degree-Based Topological Indices of $TURC_4C_8(8)$ Nanotubes

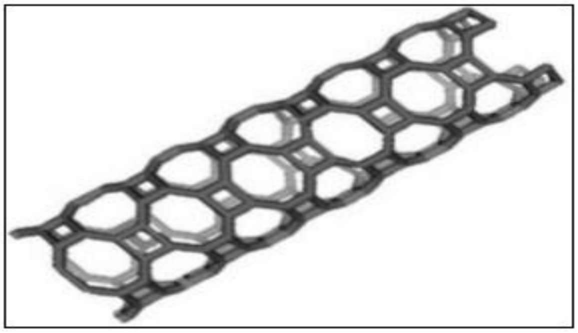

Figure 3.2

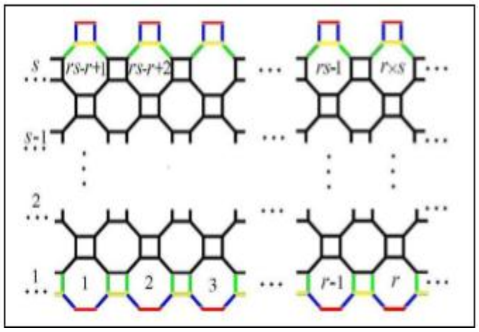

Figure 3.3

Table3.2: Summation of degrees of end points.

Summation of degrees of edge end point	$e_{(5,5)}$	$e_{(5,8)}$	$e_{(8,8)}$	$e_{(8,9)}$	$e_{(9,9)}$
Number of edges of this type	2r	4r	2r	4r	12r-11r

Theorem3.2.1: Let *G= (V, E)* be the graph of $TURC_4C_8$ (8). Then the AG_2 index of *G* are given as

$$AG_2\ (G) = \quad 16.1176r$$

Proof: To compute the $AG_2\ (G)$ index of the $TURC_4C_8$ (8).

$$AG_2(G)= \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2\sqrt{S_G\ \ u\ \ S_G\ \ v}}\right]$$

$$=e_{(5,5)}\left[\frac{5+5}{2\sqrt{5(5)}}\right]+e_{(5,8)}\left[\frac{5+8}{2\sqrt{5(8)}}\right]+e_{(8,8)}\left[\frac{8+8}{2\sqrt{8(8)}}\right]+e_{(8,9)}\left[\frac{8+9}{2\sqrt{8(9)}}\right]$$

$$+e_{(9,9)}\left[\frac{9+9}{2\sqrt{9(9)}}\right]$$

$$=2r\left[\frac{25}{2(5)}\right]+4r\left[\frac{13}{2\sqrt{40}}\right]+2r\left[\frac{16}{2(8)}\right]+4r\left[\frac{17}{2\sqrt{72}}\right]+(12r-11r)\left[\frac{18}{2(9)}\right]$$

$$=2r(2.5)+4r(1.0277)+2r(1)+4r(1.0017)+(12r-11r)\ (1)$$

$$=16.1176r$$

Theorem3.2.2: Let *G= (V, E)* be the graph of $TURC_4C_8$ (8). Then the SK_3 index of *G* are given as

$$SK_3\ (G) = 95r$$

Proof: To compute the $SK_3\ (G)$ index of the $TURC_4C_8$ (8).

$$SK_3= \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2}\right]$$

$$=e_{(5,5)}\left[\frac{5+5}{2}\right]+e_{(5,8)}\left[\frac{5+8}{2}\right]+e_{(8,8)}\left[\frac{8+8}{2}\right]+e_{(8,9)}\left[\frac{8+9}{2}\right]+e_{(9,9)}\left[\frac{9+9}{2}\right]$$

$$=2r(5)+4r(6.5)+2r(8)+4r(8.5)+(12r-11r)\ (9)$$

$$= 95r$$

Theorem3.2.3: Let *G= (V, E)* be the graph of $TURC_4C_8$ (8). Then the Sanskruti index of *G* are given as

$$S\ (G) =1016.5527r$$

Proof: To compute the Sanskruti index of the $TURC_4C_8$ (8).

$$S(G)=\sum_{u,v\in E(G)}\left[\frac{S_G\ \ u\ \ .S_G\ \ v}{S_G\ \ u\ \ +S_G\ \ v\ \ -2}\right]^3$$

$$= e_{(5,5)}\left[\frac{5(5)}{5+5-2}\right]^3 +e_{(5,8)}\left[\frac{5(8)}{5+8-2}\right]^3 +e_{(8,8)}\left[\frac{8(8)}{8+8-2}\right]^3$$

$$+\ e_{(8,9)}\left[\frac{8(9)}{8+9-2}\right]^3 +e_{(9,9)}\left[\frac{9(9)}{9+9-2}\right]^3$$

$$= 2r\left[\frac{25}{8}\right]^3 +4r\left[\frac{40}{11}\right]^3 +2r\left[\frac{64}{14}\right]^3 +4r\left[\frac{72}{15}\right]^3 +(12r-11r)\left[\frac{81}{16}\right]^3$$

$$=2r(30.5175)+4r(48.0841)+2r(95.5335)+4r(110.592)+ (12r-11r) (129.7463)$$

$$=1016.5527$$

3.3. Computing Degree-Based Topological Indices of Sierpinski Networks.

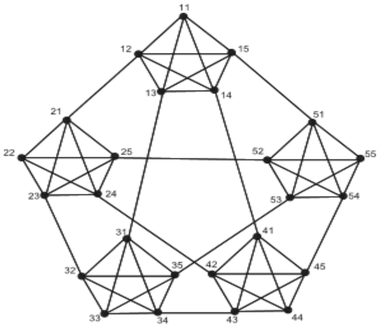

Figure 3.4

Table3.3: Edge partition of S(n,k) sierpinski network based on degrees of end vertices of each edge.

(d_u,d_v) where $u,v\in E(G)$	(k-1,k)	(k,k)
Number of edges	2k	$\frac{k^{n+1}-5k}{2}$

Theorem3.3.1: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the AG_1 index of *G* are given as

$$AG_1\ (G) = \left[\frac{2k^2-k}{\sqrt{k^2-k}}\right]+\left[\frac{k^{n+1}-5k}{2}\right]$$

Proof: To compute the AG_1 *(G)* index of the Sierpinski Networks.

$$AG_1(G) = \sum_{e,f\in E(G)}\left[\frac{d_G(e)+d_G(f)}{2\sqrt{d_G(e).d_G(f)}}\right]$$

$$=(k-1,k)\left[\frac{(k-1)+k}{2\sqrt{(k-1)k}}\right]+(k,k)\left[\frac{k+k}{2\sqrt{(k)k}}\right]$$

$$=2k\left[\frac{2k-1}{2\sqrt{k^2-k}}\right]+\left[\frac{k^{n+1}-5k}{2}\right]\left[\frac{2k}{2\sqrt{k^2}}\right]$$

$$=\left[\frac{k(2k-1)}{\sqrt{k^2-k}}\right]+\frac{k^{n+1}-5k}{2}(1)$$

$$=\left[\frac{2k^2-k}{\sqrt{k^2-k}}\right]+\left[\frac{k^{n+1}-5k}{2}\right]$$

Theorem3.3.2: Let $G= (V, E)$ be the graph of Sierpinski Networks. Then the *SK* index of *G* are given as

$$SK(G) = 4.5k^2-k+\left[\frac{k^{n+2}}{2}\right]$$

Proof: To compute the *SK (G)* index of the Sierpinski Networks.

$$SK(G)= \sum_{e,f\in E(G)}\left[\frac{d_G(e)+d_G(f)}{2}\right]$$

$$= (k-1,k)\left[\frac{k-1+k}{2}\right]+(k,k)\left[\frac{k+k}{2}\right]$$

$$= 2k\left[\frac{2k-1}{2}\right]+\left[\frac{k^{n+1}-5k}{2}\right]\left[\frac{k+k}{2}\right]$$

$$= k(2k-1)+\left[\frac{k^{n+1}-5k}{2}\right]k$$

$$= (2k^2-k)+\left[\frac{k^{n+2}-5k^2}{2}\right]$$

$$= 4.5k^2-k+\left[\frac{k^{n+2}}{2}\right]$$

Theorem3.3.3: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the SK_1 index of *G* are given as

$$SK_1\,(G) = \frac{k^{n+3} - k^3 - 4k}{4}$$

Proof: To compute the $SK_1\,(G)$ index of the Sierpinski Networks.

$$\mathrm{SK_1(G)} = \sum_{e,f\in E(G)} \left[\frac{d_G(e).d_G(f)}{2}\right]$$

$$= (k\text{-}1,k)\left[\frac{(k-1)k}{2}\right] + (k,k)\left[\frac{(k)k}{2}\right]$$

$$= 2k\left[\frac{k^2-k}{2}\right] + \left[\frac{k^{n+1}-5k}{2}\right]\left[\frac{k^2}{2}\right]$$

$$= (k^3\text{-}k) + \left[\frac{k^{n+3}-5k^3}{4}\right]$$

$$= \frac{k^{n+3} - k^3 - 4k}{4}$$

Theorem3.3.4: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the SK_2 index of *G* are given as

$$SK_2\,(G) = \frac{k^{n+3} - k^3 - 4k^2 + k}{8}$$

Proof: To compute the $SK_2\,(G)$ index of the Sierpinski Networks.

$$\mathrm{SK_2(G)} = \sum_{e,f\in E(G)} \left[\frac{d_G(e)+d_G(f)}{2}\right]^2$$

$$= (k\text{-}1,k)\left[\frac{(k-1)+k)}{2}\right]^2 + (k,k)\left[\frac{k+k}{2}\right]^2$$

$$= 2k\left[\frac{4k^2+1-4k}{2}\right]^2 + \left[\frac{k^{n+1}-5k}{2}\right] k^2$$

$$= \left[\frac{4k^3+k-4k^2}{2}\right] + \left[\frac{k^{n+3}-5k^3}{8}\right]$$

$$= \frac{k^{n+3} - k^3 - 4k^2 + k}{8}$$

Table3.4: Edge partition of graph S(n,k) where n=2 based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_u,S_v) where $u,v \in E(G)$	(k^2-k,k^2-1)	(k^2-1,k^2-1)
Number of edges	k^2-k	$\frac{k(k^n-2k+1)}{2}$

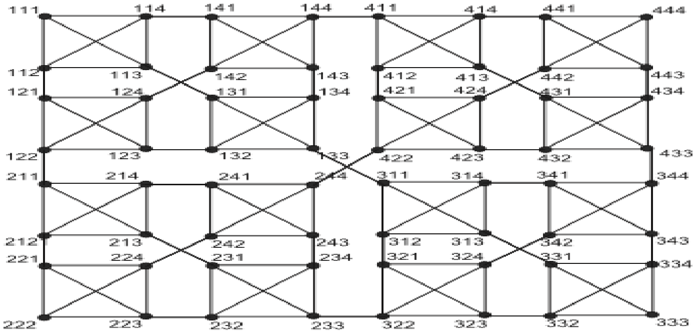

Figure 3.5

Theorem3.3.5: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the AG_2 index of *G* are given as

$$AG_2(G) = \left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k^{n+1}-2k^2+k}{2}\right]$$

Proof: To compute the $AG_2(G)$ index of the Sierpinski Networks.

$$AG_2(G) = \sum_{u,v\in E(G)}\left[\frac{Su+Sv}{2\sqrt{Su(Sv)}}\right]$$

$$= (k^2-k,k^2-1)\left[\frac{k^2-k+k^2-1}{2\sqrt{(k^2-k)(k^2-1)}}\right]+(k^2-1,k^2-1)\left[\frac{k^2-1+k^2-1}{2\sqrt{(k^2-1)(k^2-1)}}\right]$$

$$= (k^2-k)\left[\frac{2k^2-k-1}{2\sqrt{k^4-k^2-k^3+k}}\right]+\left[\frac{k(k^n-2k+1)}{2}\right]\left[\frac{2k^2-2}{2(k^2-1)}\right]$$

$$= \left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k^{n+1}-2k^2+k}{2}\right]$$

Theorem3.3.6: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the SK_3 index of *G* are given as

$$SK_3\,(G) = \left[\frac{2k^{n+3} - 2k^{n+1} + 2k^4 - 4k^3 + 4k^2}{4}\right]$$

Proof: To compute the *SK₃ (G)* index of the Sierpinski Networks.

$$\mathrm{SK}_3\,(\mathrm{G}) = \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ + S_G\ \ v}{2}\right]$$

$$=(k^2\text{-}k,k^2\text{-}1)\left[\frac{k^2 - k + k^2 - 1}{2}\right] +(k^2\text{-}1,k^2\text{-}1)\left[\frac{k^2 - 1 + k^2 - 1}{2}\right]$$

$$= (k^2\text{-}k)\left[\frac{2k^2 - k - 1}{2}\right] + \left[\frac{k(k^n - 2k + 1)}{2}\right]\left[\frac{2k^2 - 2}{2}\right]$$

$$= \left[\frac{2k^4 - 3k^3 + k}{2}\right] + \left[\frac{(2k^2 - 2)(k^{n+1} - 2k^2 + k}{4}\right]$$

$$= \left[\frac{4k^4 - 6k^3 + 2k + 2k^{n+3} - 2k^4 + 2k^3 - 2k^{n+1} + 4k^2 - 2k}{4}\right]$$

$$= \left[\frac{2k^{n+3} - 2k^{n+1} + 2k^4 - 4k^3 + 4k^2}{4}\right]$$

Theorem3.3.37: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the Sanskruti index of *G* are given as

$$S\,(G) = (k^2\text{-}k)\left[\frac{k^4 - k^3 - k^2 + k}{2k^2 - k - 3}\right]^3 + \left[\frac{k(k^n - 2k + 1)}{2}\right]\left[\frac{k^4 - 2k^2 + 1}{2k^2 - 4}\right]^3$$

Proof: To compute the Sanskruti index of the Sierpinski Networks.

$$\mathrm{S(G)} = \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ .S_G\ \ v}{S_G\ \ u\ \ + S_G\ \ v\ \ - 2}\right]^3$$

$$= (k^2\text{-}k,k^2\text{-}1)\left[\frac{(k^2 - k)(k^2 - 1)}{k^2 - k + k^2 - 1 - 2}\right]^3 +(k^2\text{-}1,k^2\text{-}1)\left[\frac{(k^2 - 1)(k^2 - 1)}{k^2 - 1 + k^2 - 1 - 2}\right]^3$$

$$= (k^2\text{-}k)\left[\frac{k^4 - k^3 - k^2 + k}{2k^2 - k - 3}\right]^3 + \left[\frac{k(k^n - 2k + 1)}{2}\right]\left[\frac{k^4 - 2k^2 + 1}{2k^2 - 4}\right]^3$$

Table3.5: n$\geq$3

(S_u,S_v) where u,v$\in$E(G)	$(k^2\text{-}k,k^2\text{-}1)$	$(k^2\text{-}1,k^2\text{-}1)$	$(k^2\text{-}1,k^2)$	(k^2,k^2)
Number of edges	k^2-k	$\frac{k(k^n-3k+2)}{2}$	k^2-k	$\frac{k(k^n-k^2-k+1)}{2}$

Theorem3.3.8: Let *G= (V, E)* be the graph of Sierpinski Networks. Then the *AG_2* index of *G* are given as

$$AG_2\,(G)=\left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{2k^4-3k^2+k}{2\sqrt{k^4-k^2}}\right]+\left[\frac{k^{n+1}-4k^2+2k-1}{2}\right]$$

Proof: To compute the *$AG_2\,(G)$* index of the Sierpinski Networks.

$$\text{AG}_2\text{(G)}=\sum_{u,v\in E(G)}\left[\frac{S_G\ \ u\ \ +S_G\ \ v}{2\sqrt{S_G\ \ u\ \ S_G\ \ v}}\right]$$

$$=(k^2\text{-}k,k^2\text{-}1)\left[\frac{k^2-k+k^2-1}{2\sqrt{(k^2-k)(k^2-1)}}\right]+(k^2\text{-}1,k^2\text{-}1)\left[\frac{k^2-1+k^2-1}{2\sqrt{(k^2-1)(k^2-1)}}\right]$$

$$+(k^2\text{-}1,k^2)\left[\frac{k^2-1+k^2}{2\sqrt{(k^2-1)k^2}}\right]+(k^2,k^2)\left[\frac{k^2+k^2}{2\sqrt{k^2(k^2)}}\right]$$

$$=(k^2\text{-}k)\left[\frac{2k^2-k-1}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k(k^2-3k+2)}{2}\right]\left[\frac{2k^2-2}{2(k^2-1)}\right]$$

$$+(k^2\text{-}k)\left[\frac{2k^2-1}{2\sqrt{k^4-k^2}}\right]+\left[\frac{k(k^n-k^2-k+1}{2}\right]\left[\frac{2k^2}{2k^2}\right]$$

$$=\left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{k^3-3k^2+2k}{2}\right]+\left[\frac{2k^4-3k^2+k}{2\sqrt{k^4-k^2}}\right]+$$

$$\left[\frac{k^{n+1}-k^3-k^2+1}{2}\right]$$

$$=\left[\frac{2k^4-3k^3+k}{2\sqrt{k^4-k^3-k^2+k}}\right]+\left[\frac{2k^4-3k^2+k}{2\sqrt{k^4-k^2}}\right]+\left[\frac{k^{n+1}-4k^2+2k-1}{2}\right]$$

Theorem3.3.9: Let *G= (V, E)* be the graph of Sierpinski Networks .Then the SK_3 index of *G* are given as

$$SK_3\,(G) = \left[\frac{k^{n+3} - 3k^3 + 2k^2}{2} \right]$$

Proof: To compute the $SK_3\,(G)$ index of the Sierpinski Networks.

$$\mathrm{SK}_3 = \sum_{u,v\in E(G)} \left[\frac{S_G\ \ u\ \ + S_G\ \ v}{2} \right]$$

$$= (k^2\text{-}k,k^2\text{-}1) \left[\frac{k^2 - k + k^2 - 1}{2} \right] + (k^2\text{-}1,k^2\text{-}1) \left[\frac{k^2 - 1 + k^2 - 1}{2} \right]$$

$$+(k^2\text{-}1,k^2) \left[\frac{k^2 - 1 + k^2}{2} \right] + (k^2,k^2) \left[\frac{k^2 + k^2}{2} \right]$$

$$=(k^2\text{-}k) \left[\frac{2k^2 - k - 1}{2} \right] + \left[\frac{k(k^2 - 3k + 2}{2} \right] \left[\frac{2k^2 - 2}{2} \right] + (k^2\text{-}k) \left[\frac{2k^2 - 1}{2} \right]$$

$$+ \left[\frac{k(k^n - k^2 - k + 1}{2} \right] \left[\frac{2k^2}{2} \right]$$

$$= \left[\frac{2k^4 - 3k^3 + k}{2} \right] + \left[\frac{(k^2 - 1)(k^3 - 3k^2 + 2k}{2} \right] + \left[\frac{2k^4 - 2k^3 - k^2 - k}{2} \right]$$

$$+ \left[\frac{k^2(k^{n+1} - k^3 - k^2 + k)}{2} \right]$$

$$= \left[\frac{2k^4 - 3k^3 + k + k^5 - 3k^4 + 2k^3 - k^3 + 3k^2 - 2k + 2k^4 - 2k^3 - k^2 - k + k^{n+3} - k^5 - k^4 + k^3}{2} \right]$$

$$= \left[\frac{k^{n+3} - 3k^3 + 2k^2}{2} \right]$$

Theorem3.3.10: Let *G*= *(V, E)* be the graph of Sierpinski Networks .Then the Sanskruti index of *G* are given as

$$S\,(G) = (k^2\text{-}k) \left[\frac{k^4 - k^3 - k^2 + k}{2k^2 - k - 3} \right]^3 + \left[\frac{k(k^2 - 3k + 2)}{2} \right] \left[\frac{k^4 - 2k^2 + 1}{2k^2 - 4} \right]^3 + (k^2\text{-}k) \left[\frac{k^4 - k^2}{2k^2 - 3} \right]^3$$

$$+ \left[\frac{k(k^n - k^2 - k + 1}{2} \right] \left[\frac{k^4}{2k^2 - 2} \right]^3$$

Proof: To compute the Sanskruti index of the Sierpinski Networks.

$$S(G) = \sum_{u,v \in E(G)} \left[\frac{S_G \; u \; S_G \; v}{S_G \; u \; + S_G \; v \; - 2} \right]^3$$

$$= (k^2\text{-}k, k^2\text{-}1) \left[\frac{(k^2 - k)(k^2 - 1)}{k^2 - k + k^2 - 1 - 2} \right]^3 + (k^2\text{-}1, k^2\text{-}1) \left[\frac{(k^2 - 1)(k^2 - 1)}{k^2 - 1 + k^2 - 1 - 2} \right]^3$$

$$+ (k^2\text{-}1, k^2) \left[\frac{(k^2 - 1)k^2}{k^2 - 1 + k^2 - 2} \right]^3 + (k^2, k^2) \left[\frac{k^2 (k^2)}{k^2 + k^2 - 2} \right]^3$$

$$= (k^2\text{-}k) \left[\frac{k^4 - k^3 - k^2 + k}{2k^2 - k - 3} \right]^3 + \left[\frac{k(k^2 - 3k + 2)}{2} \right] \left[\frac{k^4 - 2k^2 + 1}{2k^2 - 4} \right]^3$$

$$+ (k^2\text{-}k) \left[\frac{k^4 - k^2}{2k^2 - 3} \right]^3 + \left[\frac{k(k^n - k^2 - k + 1}{2} \right] \left[\frac{k^4}{2k^2 - 2} \right]^3$$

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International Journal of Current Research and Review
DOI: http://dx.doi.org/10.31782/IJCRR.2018.10165

Research Article

IJCRR
Section: Life Sciences
Sci. Journal Impact Factor: 5.385 (2017)
ICV: 71.54 (2015)

Profile of Metal Accumulation in Aquatic Macrophytes

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ABSTRACT

Industrial development coupled with population growth has resulted in the over exploitation of natural resources. Life support systems *viz*; water, air and soil are thus getting exposed to an array of pollutants especially heavy metals released by anthropogenic activities. Tolerant species of aquatic plants are able to survive and withstand the pollution stress serves as pollution indicators and as tool for phytoremediation of heavy metals is an environment clean up strategy in which green plants are employed to remove toxic contaminants and operates on the principles of biogeochemical cycling.

The aquatic plants viz; *Salvinia molesta* and *Pistia stratiotes* were used for its toxicity and profile of metal accumulation (Cadmium –Cd) from synthetic media. The test plants were cultured in a modified Hoagland solution supplemented with cadmium nitrate Cd $(NO_3)_2$. The present study focuses on Cd toxicity on morphology, biochemical parameters and bioaccumulation potential of *Salvinia* and *Pistia*. The laboratory experiments were conducted for the assay of morphological index parameters (MIP), biochemical parameters, and profile of cadmium accumulation in test plants at various concentrations viz, 0.1 ,0.5 ,1.0,1.5 & 2.0 ppm at 4 days regular intervals for 12 days exposure. The test plants show visible symptoms, like withering of roots, chlorosis, necrosis and in particular, at higher concentrations (2.0 ppm) lower leaves gets decayed. However, the lower concentrations i.e. 0.1 ppm shows normal growth. The estimation of biochemical parameters viz total chlorophyll, protein & carbohydrates of test plants showed significant increased at lower concentrations i.e. 0.1 ppm of Cd. The biochemical constituents decreased with increase in exposure concentrations i.e.0.5 to 2.0 ppm. The toxic effect Cd was directly proportional to its concentrations and exposure durations. The profile of metal accumulation by both test plants was maximum at 4 days exposure irrespective concentrations and gradually decreases at subsequent exposure concentrations and duration.

Key Words: Biochemical parameters, Cadmium, Toxicity, Accumulation, Aquatic plants

INTRODUCTION

Heavy metal pollution is a major environmental problem facing the modern world (1, 2). The global heavy metal pollution is increasing in the environment due to increases of human activities. However, it is gaining importance day by day due to its obvious impact on human health through the food chain (3). As a result of rapid growth in the industrial sectors, India is now encountering several environmental problems, especially contamination of heavy metals in water. The danger of heavy metals is aggravated by their almost indefinite persistence in the environment because they cannot be destroyed biologically but are only transformed from oxidative state or organic complex to another. In addition, they are highly toxic for both aquatic flora and fauna. The heavy metal, cadmium, is selected as toxicant for the present study because they are used in several industries in India and they are highly toxic to animals, humans and plants. Biological treatment of waste water through aquatic plants have a great potential for its purification which are effectively accumulates heavy metals (4). Aquatic macrophytes accumulates considerable amount of toxic metals and make the environment free from the pollutants. Thus, play significant role in cleaning up of environment and make the environment free from many pollutants. Many aquatic plants have been successfully utilized for removing toxic metals from aquatic environment (5). Similarly algae were also used to remove heavy metals from aquatic systems as they have capacity to accumulate dissolved metals (6, 7). The metal tolerance of plants may be attributed to different enzymes, stress proteins and phytochelatins (8). The accumulation of metals at higher concentration causes retardation of growth,

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ISSN: 2231-2196 (Print) **ISSN:** 0975-5241 (Online)
Received: 21.06.2018 **Revised:** 12.07.2018 **Accepted:** 28.07.2018

biochemical activities and also generation of –SH groups containing enzymes (9).

In the present investigation *Salvinia molesta* Mitchell and *Pistia stratiotes* L, a common aquatic floating macrophytes are used to study the effect of different concentrations of cadmium on morphology, biochemical constituents and accumulation of Cd from the experimental pond under laboratory conditions.

MATERIALS AND METHODS

Salvinia molesta and *Pistia stratiotes*, free floating aquatic plants from unpolluted water bodies is maintained in cement pots (1 m diameter) under natural conditions at a temperature 28-30^0 C. About 20 g of young healthy *Salvinia* and *Pistia* were acclimatized for two weeks in Arnon and Hoagland nutrient solution maintaining pH between 7.1-7.4. The concentrations of Cd in the polluted water are in the range of 0.1, 0.5, 1.0, 1.5 and 2.0 mg/l and tap water as a control. Morphological Index parameters (MIP) viz, root length, leaf length and breadth were observed for

12 days at interval of 4 days. Photographs of *Salvinia* and *Pistia* which were taken by using Canon's Power Shot G_2 digital camera were treated with different concentrations of copper. For the further study the plants were harvested at the end of 4, 8 and 12 days exposure and are thoroughly washed with distilled water and used for the estimation of total chlorophyll, protein and carbohydrate and also for morphological observations. Plants harvested after 48 hrs were dried at 80^0 C for 2 days for metal extraction.

The fresh test plant samples of 1g is macerated in 100 ml of 80% (v/v) chilled acetone by using pestle and mortar. The centrifuged and supernatant was used for the estimation of total chlorophyll by standard method (10) using 652 nm against the solvent (80% acetone as a blank). The protein was estimated by Lowry's method (11) using Bovine Serum Albumin (BSA) as a standard, using 660 nm and carbohydrates by phenol sulphuric acid method (12) using glucose as standard at 490 nm. Morphological characters were identified with the help of photographs, using Canon's Power Shot G_2 -digital camera.

The estimation of metal Cd in the test plant was carried out by using standard method (13). The dried and powdered 1 g plant material was digested by using mixed acid digestion method in Gerhardt digestion unit. The digested samples were diluted with double distilled water and filtered through Whatman filter paper No-44. The estimation of Cd was done by AAS (GBC 932 Plus Austrelia) with air acetylene oxidizing flame and metal hollow cathode lamp at 217.00 nm wavelength. Working standards (SISCOP-Chem-Bombay Lab) were used for the calibration of instrument.

STATISTICAL ANALYSIS

Data are presented as mean values ± SE from two independent experiments with three replicates each. Data were subjected to Two - way ANOVA to know significance between concentrations and between exposure duration for the accumulation of heavy metal (Cd). Further, Dunet's test is also applied for multiple comparisons between control and other concentrations. Two – way ANOVA test is also extended to know the significance between concentration and duration for biochemical parameters.

RESULTS

Toxicity effect of cadmium on morphology. The test plants showed luxuriant growth, shows increase in the laminal length and breadth at low concentration (0.1 ppm) in both test plants. In *Salvinia* at 0.1 ppm of Cd was found to promote laminal length by 2.166 ± 0.169, 2.200 ± 0.169 and 2.400 ± 0.094 and breadth by 2.066 ± 0.118, 2.333 ± 0.118 and 2.366 ± 0.144 at 4,8 and 12 days exposure duration. Similarly root length by 5.066 ± 0.383, 5.330 ± 0.0356 and 5.533 ± 0.381 in *Pistia* at the same concentration (0.1 ppm) shows increase in laminal length by 1.660 ± 0.027, 1.666 ± 0.027 and 1.738 ± 0.027 cm and breadth by 1.533 ± 0.027, 1.666 ± 0.047 and 1.666 ± 0.027 at 4, 8 and 12 days exposure durations respectively. Similarly, the root length by 7.000 ± 0.072, 7.130 ± 0.032 and 7.330 ± 0.027.at the same exposure duration.

However, in *Pistia* at 2.0 ppm Cd severely inhibit laminal length by 1.200 ± 0.047, 1.000 ± 0.000 and 0.700 ± 0.000 and breadth 0.833 ± 0.027, 0.813 ± 0.072 and 0.600 ± 0.072 at 4, 8 and 12 days exposure duration. Similarly root length inhibition by 4.000 ± 0.355, 3.160 ± 0.027 and 2.900 ± 0.355 at the same exposure duration.

Salvinia also shows at 2.0 ppm concentration severe inhibition of laminal length by 1.300 ± 0.047, 1.133 ± 0.072 and 1.116 ± 0.027 and laminal breadth by 1.600 ± 0.094, 1.4 ± 0.216 and 1.106 ± 0.027 at 4, 8 12 days exposure duration. Similarly root length inhibition by 2.666 ± 0.196, 1.866 ± 0.881 and 1.166 ± 0.259 cm at 4, 8 and 12 days exposure duration.(Table. 1 & 2).

Toxicity effect of Cadmium on biochemical parameters

The total chlorophyll content was very sensitive to heavy metal (Cd) toxicity. The results found that Cd at 0.1 ppm found to augment chlorophyll synthesis and was directly proportional to concentration and exposure duration in both the test plants. In *Salvinia* the chlorophyll content was increased by 3.65% (0.602 mg/g), 4.06 % (0.615 mg/g) and 4.56% (0.645 mg/g) respectively at 4, 8 and 12 days compared to control pond. Similarly in *Pistia* the chlorophyll content was increased by 0.79% (0.382 mg/g), 1.04 % (0.385 mg/g), 1.30% (0.389 mg/g) respectively at 4, 8 and 12 days compared to control pond.

However, the higher concentration of Cd found to inhibit the chlorophyll synthesis in both the test plants. The inhibition at 2.0 ppm Cd by 20.05% (0.303mg/g), 31.49% (0.261 mg/g) and 39.58 % (0.232 mg/g) significant at $P > 0.95\%$ in *Pistia* and the inhibition at 2.0 ppm Cd by 24.09% (0.441 mg/g), 29.61% (0.416 mg/g) and 34.52% (0.402 mg/g) in *Salvinia*.

Two way ANOVA represents biochemical toxicity to the test plants, concentrations were significant at $P > 0.01$ level but duration is not significant (Table. 3 & 4).

The increase in carbohydrate content of *Salvinia* at 0.1 ppm Cd by 3.44% (30.0 mg/g), 12.88% (36.0mg/g) and 13.88% (43.0mg/g) respectively. Similarly, in *Pistia* the carbohydrate content increases marginally at 0.1 ppm concentration of Cd exposure by 8.82% (37.0 mg/g), 11.42% (39.0 mg/g) and 13.15% (43.0 mg/g) respectively at 4, 8 and 12 days exposure. However, the severity of inhibition is more pronounced in *Pistia* at 2.0 ppm of Cd by 47.05% (18.0 mg/g), 62.85% (13.0 mg/g) and 74.35 % (10.0 mg/g) respectively at 4, 8 and 12 days exposure (fig.). The 2.0 ppm of Cd found to inhibit carbohydrate synthesis by 27.58% (21.0 mg/g), 43.75% (18.0 mg/g) and 65.78% (13.0 mg/g) respectively at 4, 8 and 12 days exposure in comparison to control (Fig. 1 & 2).

The protein synthesis at 0.1 ppm of Cd was promotive irrespective of exposure duration in both test plants. However, the protein content decreased at subsequent concentration and inhibition was directly proportional to the exposure duration. The 0.1 ppm of Cd promoted the protein synthesis by 2.38% (4.3 mg/g), 4.65 % (4.5 mg/g) and 6.81 % (4.7 mg/g) respectively at 4, 8 and 12 days exposure duration. Similarly for *Pistia* at 0.1 ppm shows promotive by 2.22% (4.5 mg/g), 8.33% (5.2 mg/g) and 12.24% (5.5 mg/g) respectively at 4, 8 and 12 days exposure duration (Fig. 1 & 2).

The reduction in content was observed with progressive in Cd concentration in both the test plants. The inhibition of protein content increase viz, 35.7% (2.7 mg/g), 44.18% (2.4 mg/g) and 59.09% (1.8 mg/g) was noticed in *Salvinia* at 4, 8 and 12 days exposure. Similarly in *Pistia* also at 2.0 ppm inhibition by 3.4 mg/g (24.44 %), 2.6 mg/g (45.83%) and 2.0 mg/g (59.18%) respectively at 4, 8 and 12 days exposure duration (Fig. 1 & 2).

Application of two-way ANOVA, it is found that the biochemical responses of test plants species with respect to their concentrations were significant at $P > 0.01$ level. However, exposure durations are not statistically significant (Table. 3 & 4).

Profile of metal accumulation

Fig.3 shows the concentration of Cd accumulation in *Salvinia* and *Pistia* and was directly proportional to its concentration and exposure duration. The *Salvinia* grown in experimental pond containing 0.1 ppm found to accumulate 112.050 µg/g, 130.75 µg/g and 133.75 µg/g. Similarly *Pistia* also shows metal accumulation at the same concentration by 112.50 µg/g, 130.75 µg/g and 133.75 µg/g at 4, 8 and 12 days exposure duration (Fig. 3).

However, at higher concentration (2.0 ppm) accumulation in *Pistia* by 1060.50 µg/g,1104.50 µg/g and 1125.00 µg/g and rate of accumulation in *Salvinia* also by 1270.0 µg/g, 1375.25 µg/g and 1381.00 µg/g during 4, 8 and 12 days exposure duration respectively (fig. 3).

Two way ANOVA showed that both concentration and exposure duration were significant at $P < 0.01$ level in both test plants and further Dunet's test was applied for the multiple comparison between control and different concentration treatments of test plant. From the statistical analysis it is clear that concentrations treatments are significantly differ with control (Table. 5).

DISCUSSION

Toxicity effect of Cd on morphology

1. **Morphological toxicity**: Morphometric assay is one of the quantitative tools for the assessment of toxicants measured by using Morphological Index Parameter (MIP). The rate of inhibition in the root and leaf (fronds) is directly proportional to the concentration of cadmium in both the test plants. Two way ANOVA test states the concentrations are significantly toxic at 5% level but duration is not significant. MCA test also represent maximum deviation is at higher concentration compared to control (Table 1). Both the test plants showed normal growth at their respective lower concentrations (i.e. 0.1 ppm). Similar observations were made by (14) in *Limnantherum cristatum* at 1 ppm concentration of Pb, Zn & Cr. The higher concentration of Cd (0.5 to 2.0 ppm) exhibited toxicity symptoms like chlorosis and leaf fall were observed, then brownish was occurred being marked in old leaves, respectively at higher concentration 2.0 ppm in both the test plants. Our results of toxicity symptoms of Cd at higher concentrations observed were similar to (15) and (16) and also in *Salvinia natans* (2). Sobero et. al (17) confirmed root elongation of Cd in some members of lemnaceae was found at different concentrations of Cd. The heavy metal induces morphological abnormalities in algae also (18).
2. **Toxicity effect of cadmium on biochemical parameters**: A number of heavy metals required by plants as micronutrients and they act as co-factors of enzymes

as a part of prosthetic groups and involved in a wide variety of metabolic pathway, but higher concentration of heavy metals are toxic and induces physiological and genetical changes in plants (19, 20).

In the present investigation the lower concentration of Cd promotes the synthesis of chlorophyll in *Salvinia molesta* & *Pistia stratiotes*. The enhancement of chlorophyll content from 0.602 mg/g to 0.642 mg/g in *Salvinia* & 0.379 mg/g to 0.384 mg/g in *Pistia* from 4 to 12 days exposure. The percent enhancement of chlorophyll is 4.56% in *Salvinia* & 1.56% in *Pistia* when compared to control (respective) during 12 days exposure. The stimulatory of Cd at lower concentration (0.01 to 0.4 mg/lt) was noticed in *Ceratophyllum demersum* (21). The phytochelatins (PCs) play an important role in cellular metal ion homeostasis and metal detoxification (22) and hence lower concentration of Cd shows stimulatory effect.

The Cd treatment at higher concentration decreases the chlorophyll content due to accelerated degradation of chlorophyll. In the present investigation, the inhibition varies from 0.441 mg/g to 402 mg/g in *Salvinia* and 0.303 mg g to 0.232 mg/g in *Pistia*. The inhibition is 34.52% in *Salvinia* & 34.58% *Pistia* at 12 days exposure compared to their respective control. The Cd found to inhibit general metabolic activities in many species of aquatic plants viz, Eichornia species (23) and in *Salvinia natans* (24). Inhibition activity of Cd is due to inhibition of haemobiosynthesis and chlorophyll formation by integrating with functional –SH group of enzyme involved in the biosynthesis of chlorophyll (25). Similar observation was made by (26) in *Hydrilla verticillata* at higher concentration of Pb at 20 ppm and Cd att 0.05 ppm. The decline in chlorophyll content in plants exposed to 2.0 ppm of Cd is due to i) inhibition of important enzymes associated with chlorophyll biosynthesis ii) peroxidation of chloroplast membranes resulting from heavy metal induced oxidative stress and iii) formation of metal substituted chlorophyll (27).

Carbohydrates acts as osmoregulaters which maintains water balance in plants (28). Lower concentration (0.1 ppm) of Cd increases the carbohydrate content from 30 mg/g to 36 mg/g in *Salvinia* and 37 mg/g to 43 mg/g in *Pistia* from 4 to 12 days exposure duration. The percent enhancement of carbohydrate at 12 days exposure is 13.88% in *Salvinia* and 13.55% in *Pistia* compared to respective control. However, higher concentration of Cd inhibits the synthesis of carbohydrate and vary from 21 mg/g to 3 mg/g in *Salvinia* and 18 mg/g to 10 mg/g in *Pistia* from 4 to 12 days exposure duration. The rate of carbohydrate at 2.0 ppm of Cd is 67.75% in *Salvinia* and 74.35% in *Pistia* during 12 days exposure compared to respective control. The reduction in carbohydrate content can be attributed to the reduced rates of photochemical activities. (18) and also succinic dehydrogenase (SDH) fall in cells indicate oxygen stress and energy crisis and mitochondria disturbances (29).

The lower concentration of Cd (0.1 ppm) enhance the rate of protein synthesis. The protein content vary from 4.32 mg/g to 4.7 mg/g in *Salvinia* and 4.6 mg/g to 4.7 mg/g in *Pistia* from 4 and 12 days exposure duration. The percent enhancement is 6.81% in *Salvinia* and 12.24% in *Pistia* during 12 days exposure when compared to their respective control. The stimulation of protein synthesis at lower concentration of Cd may be attired to the synthesis of stress proteins (30). The phytochelatins (PCs) are produced by Glutathione reductase (GR) and Phytochelatin Synthetase. These proteins bind and regulate the Cd and sequester the Cd toxicity and thus, plants shows metal tolerance (31).

However, the higher concentration of Cd inhibit protein metabolism in the plants. The protein content declines from 2.7mg/g to 1.8 mg/g in *Salvinia* and 3.4 mg/g to 2.0 mg/g in *Pistia* from 4 to 12 days exposure period. The percent inhibition is 59.09% in *Salvinia* and 59.18% in *Pistia* during 12 days exposure compared to respective at control. The Cd shows slight inhibitory effect 0.5 mg/lt and severe inhibition of algal growth at higher concentration in some algae (32, 18). The DNA and RNA were inhibited, rather due to blocking of _SH group or to the inactivation of RNA and DNA polymerase activity (18, 33).

Profile of metal accumulation

Heavy metal pollution of water is a major environmental concern , is increasing at alarming rate due to anthropogenic activities and is drawing attention and gaining paramanual importance due to its obvious impact on health through the food chain (1, 34). In the present investigation aquatic macrophytes viz, *Salvinia* and *Pistia* are used in accumulation. The plants exposed to concentration of cadmium, i.e 0.1 ppm found to accumulate maximum in *Salvinia* (133.75 µg/g) followed by *Pistia* (128.50 µg/g) during 12 days exposure duration. Similarly at higher concentration i.e 2.0 ppm of Cd during 12 days exposure duration shows 1381 µg/g in *Salvinia* and 1125 µg/g in *Pistia*.

Generally in our experiments it was found that the rate of accumulation is maximum at 4 days exposure irrespective of concentrations and exposure duration, however, at subsequent concentrations and exposure durations it is marginal. Similar observations were also made by (35) in *Nastutium officinale* and *Mentha aquatic* to the exposure concentrations of 0.1 and 0.5 ppm of Cd. Similar observation was made by (36) in the accumulation of Nickel in *Hydrilla verticillata* and Cd & Pb in *Salvinia cuculata* (24). The increase in the accumulation might be due to increased number of binding sites for the complexation of heavy metal ions, leading to the increased absorption, however, slow accumulation may be attributed to binding ions to the plants and establishment of equilibrium status between adsorbate and adsorbent (37, 38).

CONCLUSION

It is concluded from the findings that morphological, biochemical responses and profile of metal accumulation by *Salvinia* and *Pistia* were directly proportional to concentration of metal and maximum metal uptake was recorded at 4 days exposure and later it was marginal at subsequent concentrations and exposure durations *Pistia* stratiotes is found to be suitable candidate for toxicity evaluation. *Salvinia* molesta is the tolerant species and can be used for the remediation of heavy metals from aquatic ecosystem and environmental monitoring.

ACKNOWLEDGEMENT

The authors are thankful to the Principal, B.L.D.E.A's Degree College, Jamkhandi (India), Research and Development centre, Bharthiar University, Coimbatore. Dept. of Botany, Karnatak University Dharwad for providing necessary facilities to carry out research work. Further, the author acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also grateful to authors / editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed

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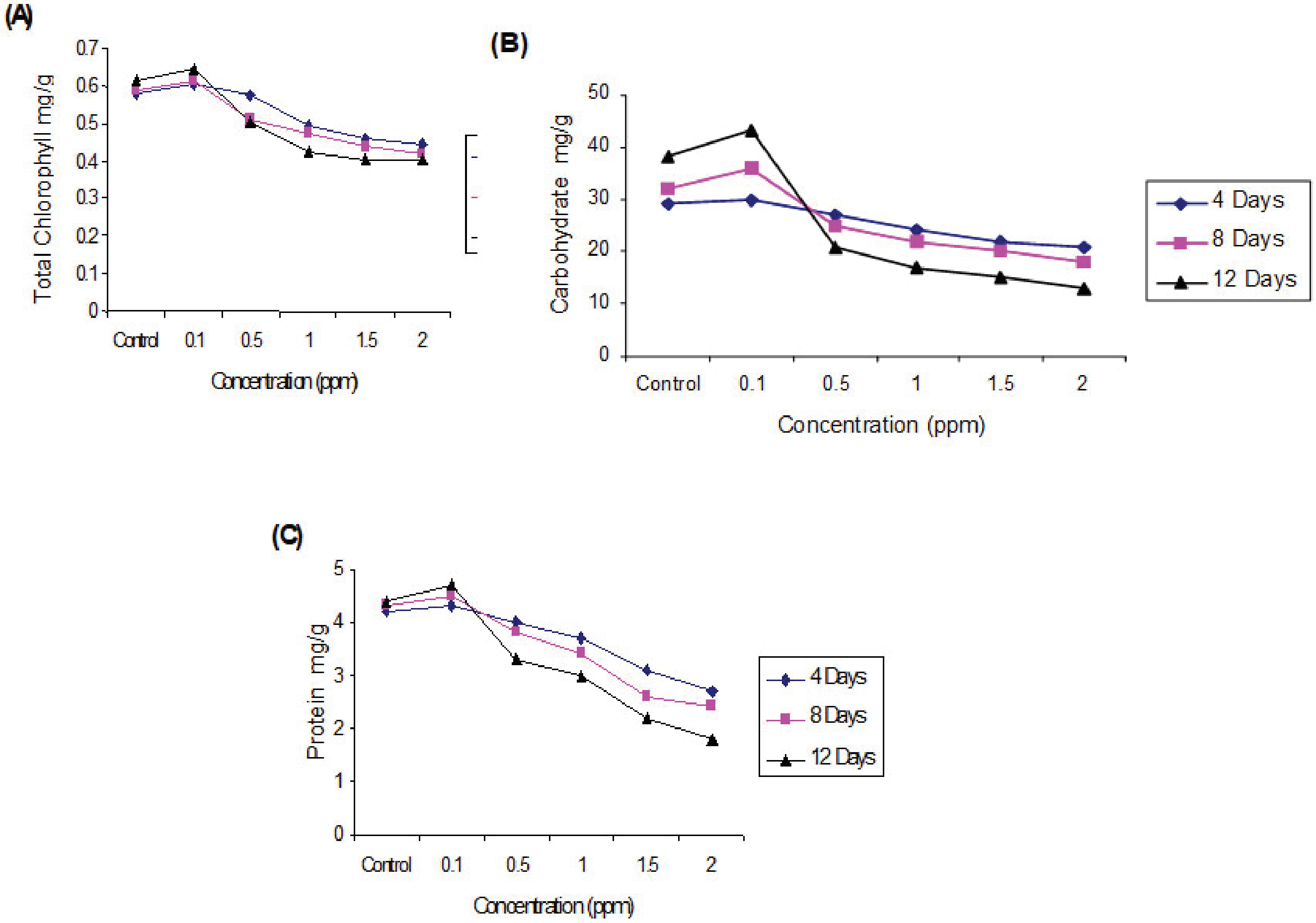


Figure 1: Biochemical effects of Cadmium on *Salvinia molesta*
(A) Total Chlorophyll (B) Carbohydrate (C) Protein

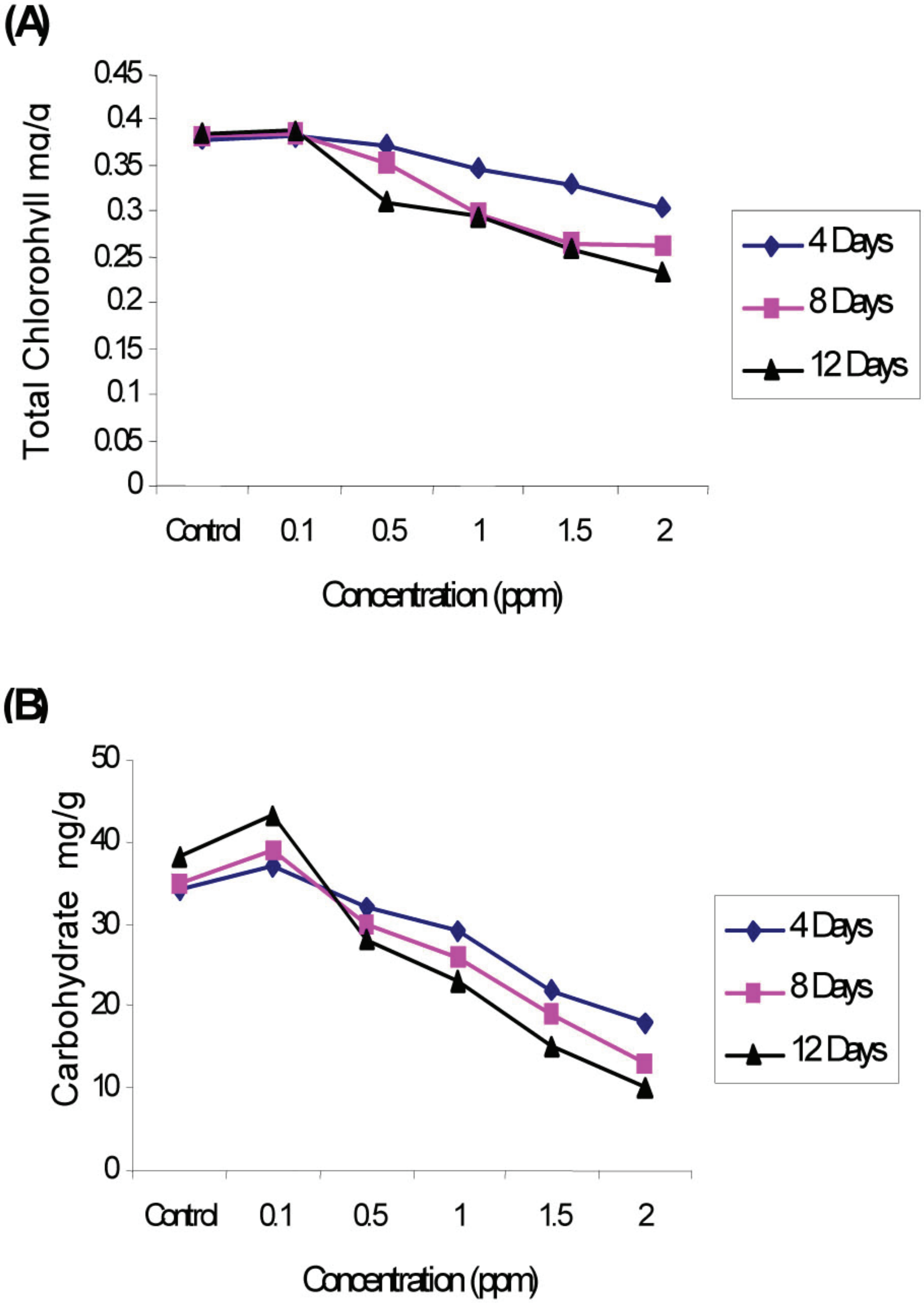
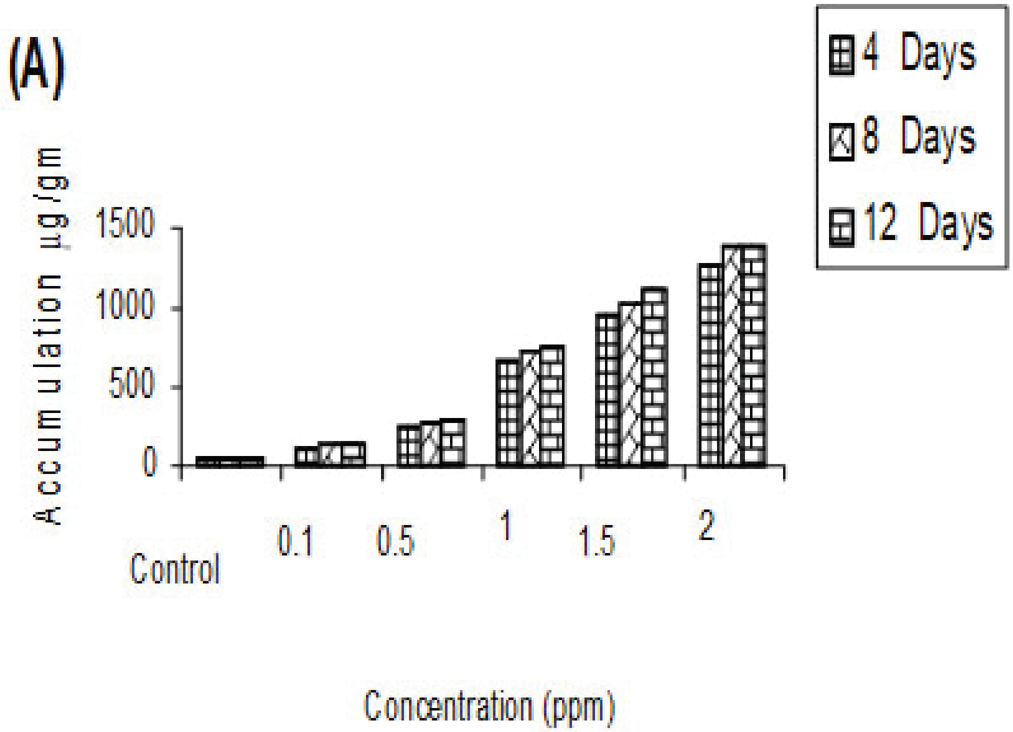


Figure 2: Biochemical effects of Cadmium on *Pistia stratiotes.*

(A) Total Chlorophyll (B) Carbohydrate (C) Protei



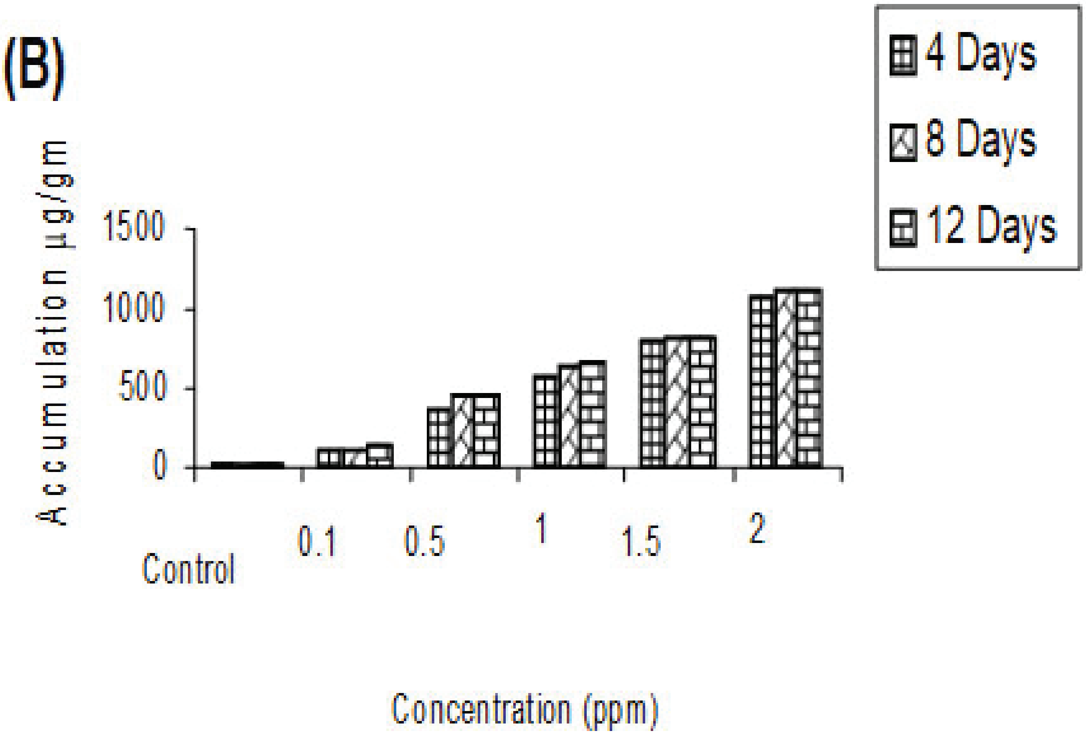


Figure 3: Accumulation profile of Cadmium by aquatic macrophytes.

(A) *Salvinia* (B) *Pistia*

Table 1: Effect of Cadmium on morphology of *Salvinia molesta*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	4.400 ± 0.309	4.533 ± 0.212	4.766 ± 0.232	1.766 ± 0.027	2.000 ± 0.047	1.766 ± 0.027	2.000 ± 0.047	2.030 ± 0.047	1.900 ± 0.047
0.1	5.066 ± 0.383	5.330 ± 0.035	5.533 ± 0.381	2.166 ± 0.178	2.066 ± 0.118	2.200 ± 0.169	2.333 ± 0.118	2.400 ± 0.094	2.366 ± 0.144
0.5	4.366 ± 0.178	4.166 ± 0.144	4.066 ± 0.136	1.933 ± 0.151	1.966 ± 0.072	1.866 ± 0.136	1.900 ± 0.081	1.732 ± 0.118	1.800 ± 0.047
1.0	4.066 ± 0.136	3.866 ± 0.151	3.733 ± 0.098	1.733 ± 0.108	1.666 ± 0.054	1.666 ± 0.054	1.500 ± 0.047	1.533 ± 0.022	1.366 ± 0.027
1.5	4.000 ± 0.047	3.300 ± 0.205	2.333 ± 0.276	1.666 ± 0.054	1.633 ± 0.151	1.600 ± 0.124	1.433 ± 0.151	1.533 ± 0.027	1.266 ± 0.072
2.0	2.666 ± 0.196	1.866 ± 0.381	1.166 ± 0.259	1.300 ± 0.047	1.600 ± 0.094	1.133 ± 0.072	1.4 ± 0.216	1.116 ± 0.027	1.106 ± 0.027

Values are expressed in cms
Mean values ± Standard Error

Table 2: Effect of Cadmium on morphology of *Pistia stratiotes*

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	6.100 ± 0.047	6.160 ± 0.072	6.300 ± 0.124	1.400 ± 0.047	1.330 ± 0.027	1.466 ± 0.027	1.366 ± 0.027	1.476 ± 0.027	1.376 ± 0.047
0.1	7.000 ± 0.072	7.130 ± 0.032	7.330 ± 0.027	1.660 ± 0.027	1.533 ± 0.027	1.666 ± 0.027	1.533 ± 0.047	1.738 ± 0.027	1.666 ± 0.027
0.5	6.360 ± 0.072	6.260 ± 0.072	6.100 ± 0.047	1.500 ± 0.047	1.333 ± 0.027	1.500 ± 0.047	1.333 ± 0.027	1.333 ± 0.027	1.111 ± 0.027
1.0	4.766 ± 0.047	4.600 ± 0.08	4.290 ± 0.047	1.400 ± 0.047	1.333 ± 0.027	1.400 ± 0.047	1.333 ± 0.027	1.300 ± 0.027	1.212 ± 0.02
1.5	4.533 ± 0.072	4.466 ± 0.151	3.240 ± 0.047	1.333 ± 0.027	1.066 ± 0.720	1.200 ± 0.00	1.060 ± 0.072	1.000 ± 0.00	1.100 ± 0.027
2.0	4.000 ± 0.355	3.160 ± 0.027	2.900 ± 0.355	1.200 ± 0.047	0.833 ± 0.027	1.000 ± 0.00	0.813 ± 0.072	0.700 ± 0.00	0.600 ± 0.072

Values are expressed in cms
Mean values ± Standard Error

Table 3: Two way ANOVA for biochemical effects of Cadmium on *Salvinia molesta*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	29.987**	8.057**	27.085**
F- value (between duration)	1.585	0.088	3.333

** Significant at P < 0.01 level

Table 4. Two way ANOVA for biochemical effects of Cadmium on *Pistia stratiotes*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	17.647**	32.381**	13.658**
F- value (between duration)	6.166	1.0.65	1.850

**Significant at P < 0.01 level

Table 5: Two way ANOVA with Dunet's test for multiple comparison for accumulation of Cadmium by aquatic macrophytes

	Salvinia	Pistia
F-Value (between concentration)	733.87**	1820.94**
F- value (between duration)	8.13**	13.27**
Dunet's Value	53.60	26.57
Control V/s 0.1 ppm	79.25	97.08
Control V/s 0.5 ppm	225.83	399.41
Control V/s 1.0 ppm	662.00	600.91
Control V/s 1.5 ppm	982.41	785.91
Control V/s 2.0 ppm	1295.66	1074.25

** Significant at $P < 0.01$ level

REVIEW OF RESEARCH
IMPACT FACTOR : 5.2331(UIF) UGC APPROVED JOURNAL NO. 48514 ISSN: 2249-894X
VOLUME - 7 | ISSUE - 8 | MAY - 2018

ROLE OF EDUCATION IN OVERALL DEVELOPMENT OF KARNATAKA: AN OVERVIEW

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ABSTRACT

Education as a catalyst plays a vital role in increasing the speed of the social change. In class based society like India it is evinced that there are social, economical and political disparities. Education plays prominent role in minimizing these disparities. The present paper is based on secondary sources. This paper emphasizes on the literacy rates of the districts in Karnataka state, it is noted that about 12 districts of Karnataka state has a literacy rate above 75.60 %. It is observed that during the decade from 2001 to 2011 there is significant growth in literacy rates in all the districts of Karnataka. The Teacher –Student ration which was 34 in 2001 has decreased to 26 in 2013. Despite of this, the Teacher-Student ration is less than prescribed standard. It can be considered as one of the remarkable progress. The credit of it goes completely too Universal Education Campaign (Sarva Shikshana Abhiyana). It was noticed that, during the period from 2000 to 2013 there was slight increase in disparities between the districts. The index recorded the the rise of 0.74 %. It is observed that, in all the districts, till 2013 there is a decrease in the rate of bringing back the school dropouts students back to the school. Therefore, it is understood that education sector has to become much more effective and adopt various educational developmental programmes in order to achieve equal growth in all the regions.

KEY WORDS: *Literacy, Economy, Development, Regionalism, Ratio, Children, Teachers, inequality, Education, Disparity.*

1. INTRODUCTION:

It is observed that there exists a mutual relation between the educational progress and social change. Kerala state is an excellent example for this. The education sector in Karela has played a vital role in eradicating the caste, class, and gender based cultural disparities. But comparatively the North Indian states lagging in education have not achieved academic progress. If the economic programmes development like, economical growth opportunities, economic improvements and health which empowers the public are not efficiently adopted it is indeed impossible to empower the people. If the education is viewed in the regional perspective it is evident that from the 1991, 2001 and 2011 census that education rate of Karnataka has considerably increased which is matter of contention. Apart from the increase in the education rate, the difference in education rate between men and women has also considerably decreased in these decades. Despite the state enjoys overall increase in education rate however, there is regional disparity in the education sector which is very unfortunate and alarming aspect on the part of the state.

Education is firm platform for both economical and physical development. Education is the main source of human evolution. Since India is an agriculture based country, the people of India do not know much apart from agricultural activities. It is indeed a tough task to provide skill development training, create scientific awareness to the people under the clutch of poverty since from several centuries. The wellness of the public is the main objective of the democratic system, as the democratic system widened it was implicit that the communication of education became one of the important duties. During the pre-independence and later farter the concept of welfare state the public education gained importance. Therefore an Amendment 21(A) was made to the 86th Article of Indian constitution. Wherein, the education to the children between the age group of 6 to 14 was made compulsory and fundamental right. Later the Education right introduced in 2010 further strengthened the education sector.

2. REVIEW OF LITERATURE:

D.M. Nanjundappa Report (2002): On the basis of progress of democracy there was a voice for the separate state, in this background C.M. Krishna then Chief Minister of Karnataka framed a committee “Regional Disparity Resolving Committee” under the Chairmanship of Dr. D.M. Nanjundappa in October 2000. Dr. D.M. Nanjundappa committee established with the objective of resolving the regional disparity analyzed the major aspects like population, agriculture, trade, industries, roads, education, irrigation, electricity, appointments and other various aspects and selected 35 indexes. The committee analyzed the data using these indices and submitted its final report to the government in 2002.

Venkatesh and Saroja et.al. (2006), this article includes several articles written by various experts. More importantly, the agriculture, irrigation, literacy, economy and social development, literacy pertaining to Hyderabad Karnataka region is reviewed. Further this article throws light on the Nanjundappa committee report and calls for providing special status to Hyderabad Karnataka region. The article also throws light on the various movements witnessed in Hyderabad Karnataka region.

3. OBJECTIVES OF THE STUDY:

To analyze the district wise educational development in the Karnataka state.

4. RESEARCH METHODOLOGY:

The present study completely includes secondary sources. The data is collected from District at a glance and Dr. D.M. Nanjundappa Report.

4.1. statistical tools:

The statistical tools like percentage; Coefficient of Variation (CV) is used in this study.

5. ANALYSIS AND INTERPRETATION:

District wise educational development in Karnataka State (Results and Discussion)

The literacy rate of people in the nation plays a vital role in the development of the nation. Only people with quality education can ensure social change and economical development. Though constitution of India has provisioned free and compulsory education to the children of the age group of 6 to 14, even today the education status in some of the states is still lagging. Karnataka state is no excuse in this matter. The educational development in the state can be understood from various educational disparity indexes. Literacy rate, the student and teacher ratio in the primary school, the average number of school dropout students in the age group of 6 to 14 years are the various indexes used for analyzing the educational status.

Table No.1. Literacy Rate (Percentage)

Division	District	2001	2011	Difference
Banglore Division	Bengluru Urban	83.9	87.7	3.76
	Bengluru Rural	65.0	77.9	12.93
	Chikkaballapur	60.2	69.8	9.60
	Chitradurga	64.9	73.7	8.83
	Davanageri	67.7	75.7	8.07
	Kolar	63.1	74.4	11.25
	Ramanagar	64.6	69.2	4.59
	Shivamogga	74.9	80.4	5.59
	Tumakur	67.2	75.1	7.95
Mysore Division	Chamarajanagar	51.3	61.4	10.17
	Chikkamangaluru	72.6	79.2	6.62
	Dakshina Kannada	83.5	88.6	5.10
	Hasana	68.8	76.1	7.32
	Kodagu	78.2	82.6	4.44
	Mandya	61.2	70.4	9.19
	Mysore	63.7	72.8	9.10
	Udapi	79.9	86.2	6.37
Belagavi Division	Bagalkot	57.8	68.8	11.01
	Belagavi	64.4	73.5	9.06
	Dharwad	71.9	80.0	8.13
	Gadag	66.3	75.1	8.85
	Haveri	68.1	77.4	9.31
	Uttara Kannada	76.6	84.1	7.47
	Vijayapur	57.5	67.1	9.69
Gulburga Division (Hydrabad Karnataka)	Bellary	58.0	67.4	9.39
	Bidar	62.0	70.5	8.53
	Gulburga	50.7	64.9	14.20
	Koppal	55.0	68.1	13.07
	Raichur	49.5	59.6	10.02
	Yadgir	37.4	51.8	14.40
	State	67.0	75.6	8.56
	Co-efficent Variations	16.12	11.34	4.78

Source: Dr. D.M.Nanjudappa Report-2002 And District At A Glance 2013-14 (All the Districts), Karnataka At A Glance 2015-16.

As indicated in Table 1, the literacy rate is most general and important index. This index counts and examines the literacy rate. Though Karnataka state is committed and aims to obtain complete literacy, the literacy rate in Karnataka is still lagging. The table throws light on the literacy rates at the various districts of Karnataka state. As per 2011 census the total literacy rate in Karnataka state was 75.60 %. It is evident from the data that still about 25% of the population of Karnataka state are illiterates. Further the Eleventh Five Year plan aims to achieve 85% literacy rates by the time of end of the plan. But when the present literacy rate is examined it appears to be impossible task to achieve 85% literacy rate. Presently, it is essential and need of the hour to increase the literacy rate in Karnataka. On comparison of the literacy rates at the different districts of the state it is evident that, the literacy rates are not similar throughout the state. From the 2001 and 2011 census it is evident that in 2011 the literacy rate has improved by 4.78 % from that of 2001 census.

It is evident from table that the in about more than 12 districts of the state the literacy rate is more than 75.60 %. It is observed that there is a considerable amount of improvement in the literacy rate during the decade between 2001 and 2011. Yadagir district has a recorded 14.04 % percent rise, a maximum literacy growth in the state. Despite of this the literacy rate at Yadgir district when compared to all the districts is just 51.83%. Further during the decade between 2001 and 2011 the rise in the literacy rate in Kalaburgi and Koppal district is 14.20 % and 13.07 % respectively. When the data of 2011 is reviwed, as per the report of Dr. Nanjundappa committee report the literacy rates at various backward districts of Karnataka have increased by 10%. This is considered one of the positive moves toward education. Further, Dakshin Kannada, Bengaluru city and Udupi districts of Karnataka state attains first three positions respectively with respect to the literacy rate index. When these facts and figures are analyzed it is evident that the literacy rates in the districts of Hyderabad Karnataka regions are low when compared to other districts of Karnataka state.

Table No.2. 1 to 10 the Class Student and Teachers Ratio

Division	District	2000	2013	CAGR
Banglore Division	Bengluru Urban	65	22	-7.99
	Bengluru Rural	28	19	-2.86
	Chikkaballapur	31	32	0.36
	Chitradurga	33	23	-2.70
	Davanageri	34	22	-3.17
	Kolar	31	26	-1.29
	Ramanagar	26	20	-1.91
	Shivamogga	28	22	-1.73
	Tumakur	28	23	-1.51
Mysore Division	Chamarajanagar	35	28	-1.78
	Chikkamangaluru	25	17	-2.99
	Dakshina Kannada	38	27	-2.69
	Hasana	26	18	-2.79
	Kodagu	26	22	-1.24
	Mandya	33	33	0.05
	Mysore	35	23	-3.18
	Udapi	37	23	-3.45
Belagavi Division	Bagalkot	40	30	-2.28
	Belagavi	38	27	-2.55
	Dharwad	32	28	-0.97
	Gadag	37	26	-2.70
	Haveri	36	25	-2.80
	Uttara Kannada	25	21	-1.29
	Vijayapur	38	29	-2.00
Gulburga Division (Hydrabad Karnataka)	Bellary	42	28	-3.07
	Bidar	42	26	-3.75
	Gulburga	42	40	-0.35
	Koppal	45	68	3.26
	Raichur	44	27	-3.73
	Yadgir	44	32	-2.44
	State	34	26	-1.90

	Co-efficent Variations	23.44	34.22	10.78

Source: Dr. D.M.Nanjudappa Report-2002 And District At A Glance 2013-14 (All the Districts),
Note: Compound Annual Growth Rate (CAGR)

As per Table 2, the student -teacher ratio of 1st to 10th schooling also forms one of the important indexes. The ratio of teachers available according to the proportion of students as per main literacy ratio is suggested in the table. As per the right to education article the prescribed Pupil-Teacher Ratio is 30:1. Higher Primary school has prescribed Pupil Teacher Ratio (PTR). The Pupil-Teacher Ratio (PTR) in various district of Karnataka is shown in Table-2. The PTR which was recorded 34 in 2001 reduced to 26 in 2013. This PTR value is less than the prescribed value. Therefore it can be considered as the remarkable achievement. The credit of this achievement goes to Universal Education Movement (Sarva Shikshana Abhiyana). Further the value of PTR recorded in 25 districts of Karnataka is 25 which is even less than 30. Gulbarga, Koppal, Yadagiri, Mandya and Chikkaballapur districts of Karnataka records PTR value more than 30. At one hand the PTR value is decreasing at some districts whilst on the other hand the disparity between inter districts has considerably increased by 10.78 points. 68:1 the highest value of PTR is recorded in Koppal district. Likewise lowest value of PTR is recorded in Chikkamagalur. The difference of PTR values between the highest and lowest recorded districts is 51 points. Therefore it is essential to reduce the inter district disparity.

Table: 3: The percentage of School dropouts between the age group of 6 to 14

Division	District	2000	2013	Difference
Banglore Division	Bengluru Urban	2.72	2.39	-0.33
	Bengluru Rural	4.4	0.11	-4.29
	Chikkaballapur	12.2	1.52	-10.68
	Chitradurga	7.5	1.96	-5.54
	Davanageri	7.7	1.70	-6.00
	Kolar	9.81	1.78	-8.03
	Ramanagar	6.81	0.09	-6.72
	Shivamogga	6.1	0.17	-5.93
	Tumakur	4.5	1.08	-3.42
Mysore Division	Chamarajanagar	9.14	1.97	-7.17
	Chikkamangaluru	6.78	0.28	-6.50
	Dakshina Kannada	1.76	0.57	-1.19
	Hasana	5.11	0.80	-4.31
	Kodagu	8.52	2.24	-6.28
	Mandya	4.27	0.07	-4.20
	Mysore	9.01	1.92	-7.09
	Udapi	1.1	0.78	-0.32
Belagavi Division	Bagalkot	13.22	1.99	-11.23
	Belagavi	8.46	1.49	-6.97
	Dharwad	8.54	0.31	-8.23
	Gadag	10.11	2.34	-7.77
	Haveri	8.4	0.21	-8.19
	Uttara Kannada	6.89	0.92	-5.97
	Vijayapur	17.32	2.38	-14.94
Gulburga Division	Bellary	16.75	2.81	-13.94
	Bidar	12.41	1.68	-10.73

(Hydrabad Karnataka)	Gulburga	24.37	3.42	-20.95
	Koppal	21.95	3.21	-17.74
	Raichur	26.73	1.13	-25.6
	Yadgir	35.67	4.83	-30.84
	State	10.03	1.68	-8.35
	Co-efficent Variations	73.71	74.45	

Source: Dr. D.M.Nanjudappa Report-2002 and District at a Glance 2013-14 (All the Districts).

Table 3: fetches the percentage ratio of the School dropouts between the age group of 6 to 14. The main objective of the Universal Education Scheme (Sarva Shikshana Abhiyana) is to reduce the number of School dropouts. Sarva Shikshana Abhiyan took up the survey all over Karnataka in 2000 and reported that 8,13,563 children between the age group of 6 to 14 are school dropouts. Sarva Shikshana Abhiyana took up various programmes and succeeded in bringing 90% of the school dropout children back to school. Therefore only 10% of the children between the age group of 6 to 14 are remained as school dropouts. In Karnataka during 2013 the numbers of school dropout between the age group of 6 to 14 further reduced by 1.68%. During the period between 2000 and 2013 there is a slight rise in the disparity value between the inter districts. There is a rise of 0.74% in the disparity index level between the inter districts. Till 2013 there is considerable decrease in bringing back the school dropouts children to the school. It is observed that, the school dropout children ratio in Yadagir district of Karnataka is 4.83. When the school dropout ratio is compared with other districts it is noticed that in Yadgir district the school dropout children ratio has decreased by 30.84 points during this period. It is also noticed that the ratio of the school dropout children in this region is also quite high. Further, it is also observed that school dropouts' children at other backward districts of Karnataka have also considerably decreased. Likewise, it is observed that the school dropout children ratio recorded in Raichur, Kalaburgi and Koppal is 25.60 points, 25.90 points and 17.74 points respectively. When all these aspects are reviewed it is evident that the disparity still prevails in the backward districts. Therefore it is indeed necessary for the government to implement new programmes to eradicate disparity and attain equal development.

The present study throws light on the present status of education system in various districts of Karnataka state. There is a disparity in terms of literacy rate, school dropout children and Pupil-Teacher Ratio (PTR) amongst the different districts of the state. Though disparity prevails the index evinces development. As the literacy rate has considerably increased it can be said that education sector is been developing. Government has to give priority to the regions which are termed as backward regions on the basis of fundamental infrastructure index. When the disparity in the development of education sector in the districts of Karnataka is observed it is evident for the government to adopt micro and intensive guidelines to resolve the disparity issue.

6. CONCLUSION:

It is indeed impossible to rule out that Education sector in Karnataka has made a remarkable progress in the last six decades after the state became reunited on the basis of common language speaking region. But if at all the governments had adopted equality in the distribution of infrastructure, atmosphere and staff required for the development in the backward regions, today the backward regions would have also achieved much more progress. Though the facts and figures have considerably progressed, there is indeed requirement of hard work and grants for achieving qualitative progress. While appointing teachers the backward regions are to be prioritized. Likewise, when providing various infrastructure facilities priority is to be given to the backward region.

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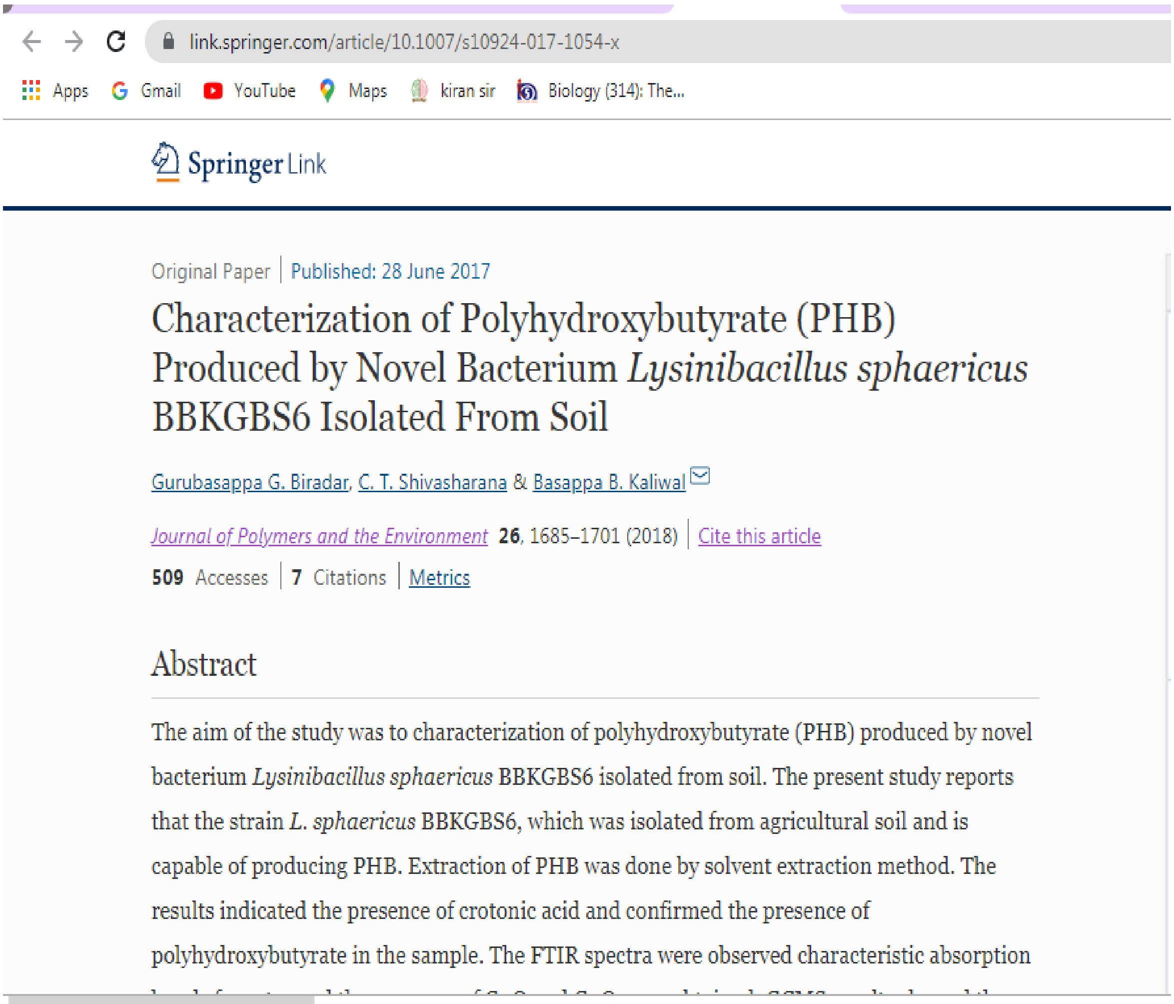

Original Paper | Published: 28 June 2017

Characterization of Polyhydroxybutyrate (PHB) Produced by Novel Bacterium *Lysinibacillus sphaericus* BBKGBS6 Isolated From Soil

Gurubasappa G. Biradar, C. T. Shivasharana & Basappa B. Kaliwal

Journal of Polymers and the Environment **26**, 1685–1701 (2018) | Cite this article

509 Accesses | **7** Citations | Metrics

Abstract

The aim of the study was to characterization of polyhydroxybutyrate (PHB) produced by novel bacterium *Lysinibacillus sphaericus* BBKGBS6 isolated from soil. The present study reports that the strain *L. sphaericus* BBKGBS6, which was isolated from agricultural soil and is capable of producing PHB. Extraction of PHB was done by solvent extraction method. The results indicated the presence of crotonic acid and confirmed the presence of polyhydroxybutyrate in the sample. The FTIR spectra were observed characteristic absorption

Journal of Pharmaceutical Research International

21(6): 1-11, 2018; Article no.JPRI.39532
ISSN: 2456-9119
(Past name: British Journal of Pharmaceutical Research, Past ISSN: 2231-2919, NLM ID: 101631759)

Isolation and Identification of Bacterial Strains Able to Biopolymer Polyhydroxybutyrate (Phb) Production from Soil of Al-Kharj Probes, Saudi Arabia

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Author's contribution

The sole author designed, analyzed and interpreted and prepared the manuscript.

Article Information

DOI: 10.9734/JPRI/2018/39532
Editor(s):
(1) Barkat Ali Khan, Department of Pharmaceutics, Gomal University, Dera Ismail Khan, Pakistan.
(2) R. Deveswaran, Professor, M. S. Ramaiah College of Pharmacy, Bangalore, India.
Reviewers:
(1) Merih Kivanç, Anadolu University, Turkey.
(2) Katarzyna Leja, Poznań University of Life Sciences, Poland.
(3) Nur Ceyhan Güvensen, Muğla Sıtkı Koçman University, Turkey.
Complete Peer review History: http://www.sciencedomain.org/review-history/23891

Original Research Article

Received 20th January 2018
Accepted 23rd March 2018
Published 30th March 2018

ABSTRACT

Polyhydroxyalkanoates (PHAs), which is produced by several bacteria, is a biodegradable polymer that has many industrial and medical applications such as heart valves, scaffold, suture and drug delivery. The aim of the present study is to isolate and identify the bacteria producing polyhydroxybutrate (PHB) from the soil sample of Al-Kharj, south of Riyadh, Kingdom of Saudi Arabia. After staining the bacterial isolates with Nile red stain, the only lighted isolates were selected for further identification. The strongest florescent strain (G-4) was identified by morphological and biochemical tests as *Bacillus* sp. For further confirmation, PHB was extracted from the G-4 isolate by three different methods of extraction and analyzed by IR. The effect of different conditions on PHB produced by bacterial isolate (G-4) including carbon sources, nitrogen sources, incubation temperatures, pH and incubation periods were studied. The highest production of PHB was observed with cultural media containing 8% of date palm syrup (Khalas) at the pH of

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7.2. These results show that *Bacillus* species identified in soil sample of Al-Kharj produced highest concentration of PHB by using date palm syrup as a carbon source that can substantially reduce substrate and production costs of PHB.

Keywords: Polyhydroxybutrate; date palm syrup; nile red; PHA producer; Bacillus sp.

1. INTRODUCTION

Plastics are synthetic polymers which have wide applications ranging from packaging, domestic, aquatic and architectural industries. The synthetic plastics are characterized by light weight, and durability. Due to their non-biodegradable nature, they accumulate in the environment causing global environmental pollution [1]. Now need arises to develop biodegradable plastics that will opened a way for new strategies for waste management. Polyhydroxybutyrate (PHB) is one of the most biodegradable and biocompatible thermoplastic synthesized by many microorganisms, collectively called polyhydroxyalkanoates (PHAs) [2,3]. These biodegradable plastics are considered the best solution for solving the environmental pollution problems by replacing conventional plastics industries [4]. Because of their biological nature, PHAs completely hydrolyzes into water and carbon dioxide by different microorganisms found in soil [5,6]. Because of its biodegradable characteristics, these compounds can be used as biodegradable carriers for long-term dosage of drugs, medicines, hormones, insecticides and herbicides [7]. They are also used as osteosclerotic stimulants owing to their piezoelectric properties, in bone plates, surgical sutures and blood vessel replacements [8]. PHB might be synthesized by wide range of Gram positive and negative bacteria from different genera [9]. These PHB producing bacteria should have optimal cultural conditions including high concentration of carbon source and limited concentration of nitrogen, phosphorus, sulphur and/or trace elements [10]. In fact, to commercialize PHAs, substantial effort has been devoted to reducing the production cost through the development of bacterial strains and more efficient fermentation/recovery processes because the price of the substrate has the largest influence on the production cost of PHA [11]. The flora of microorganisms in Al-Kharj area are not utilized, therefore, this study will utilize these natural resources for production of useful biodegradable biopolymer and using inexpensive resources available in Saudi Arabia such as date palm syrup as alternate carbon source for production of PHB from the isolate (G-4).

2. MATERIALS AND METHODS

2.1 Isolation and Selection of PHB-Producing Bacteria

Soil samples collected from different localities in Al-Kharj were used for isolation of the PHB producing bacteria according to the method of Bormann et al. [12] as follows. 1.0 g of sample was serially diluted in sterile distilled water and plated onto nutrient agar plates and incubated at 30ºC for 24 hours. Various colonies of different morphologies were individually picked and subcultured 3-4 times on nutrient agar plates. The bacterial colonies were streaked on nutrient agar slants, incubated at 30ºC overnight and then stored at 4ºC for further use. Screening test for the PHB production of the isolated strains was performed using Nile-Red [9-diethylamino-5H-benzo α- phenoxazine-5-one. (Sigma)] staining approach [13]. 20 µl of Nile red stock solution was spread onto sterilized LB agar plates to reach a final concentration of 0.5 µg Nile Red/ml medium. The plates were incubated after inoculation overnight at 35°C. The plates were then exposed to ultraviolet light at 300 nm to detect the accumulation of the PHB. The lighted plates were recorded positives PHB production and these isolates were selected for the subsequent identification [14].

2.2 Extraction of Date Syrup with Water

Date pulp (100 gm) of date fruits (*Phoenix dactylifera* L.) of Khalas variety at the tamr stage of maturity put in an erlenmeyer flask (1 L) and water were added at 1:5 ratios. The date pulp/water sample was blending using a hand-held blender (Phillips, Holland). The pH was adjusted to 6.0 ± 0.2. The sample, in triplicate, was placed in water bath at 70ºC for 2 h. After heating the slurry was filtered through a cheese cloth with a hand press to remove large impurities and insoluble matters then centrifuged at 8000 g for 10 min, and the supernatant was decanted.

2.3 Infra-Red (IR) Spectroscopic Analysis of PHB

The extracted polymer was qualitative analyzed by Fourier transform infrared spectroscopy (FTIR) (FT-IR - 4100, Jasco, Europe) to determine its functional groups contents. According to the method of Gopi et al. [15] 1 mg of each of the PHB standard and the extracted were dissolved in 5 ml of chloroform, then chloroform was evaporated and KBr pellet. IR spectra were recorded in 4000 cm-1 to 400 cm- 1 range.

2.4 Optimization of Cultural Conditions for Maximum PHB Production

The production of PHB from the positive isolate was affected by the culture conditions. Therefore, different media (LB) medium: 16 g trypton, 10 g Yeast extract and 10 g NaCl [16], (SG) medium: 25%, (w/v): NaCl, 2%(w/v): $MgSO_4.7\ H_2O$, 0.2%, (w/v): KCl, 3%, (w/v): Tri Sodium citrate, 1% (w/v): Yeast extract and 0.75%, w/v): Casmino acids [16] and Mineral Salt Medium (MSM): 0.05% (w/v) NH_4Cl, 0.74%(w/v) KH_2PO_4, NaCl, 2.46 g $MgSO_4\ 7H_2O$, 82 mg EDTA, 1.25 mg $ZnCl_2$, 0.75 mg Mn Cl_2, 7.5 mg H_3BO_3, 5 mg $CoSO_4\ 7\ H_2O$, 0.25 mg $CuCl_2\ 7H_2O$, 0.75 mg $Na_2MoO_4.\ 2H_2O$, 0.5 mg $NiCl_2.\ 6\ H_2O$ and 7.0 mg $FeCl_3.\ 6\ H_2O$ [17] were used with different cultivation conditions [18]. Minimal salts medium (MM): 4 g $NaNO_3$, 1.5 g KH_2PO_4, 0.5 g Na_2HPO_4, 0.001 g $FeSO_4.7H_2O$, 0.2 g $MgSO_4.7H_2O$, and 0.01 g $CaCl_2$ [17] was used as (control) in all experiments in this work.

For optimization of the best incubation periods to production of PHB, different incubation time (24h, 48h, 72h) were studied. For pH optimization, culture was incubated in carbon rich nutrient medium with different pH range from 6.5 to 8.5. Each culture was taken from different flask and PHA production was determined. Effect of media ingredients like carbon, phosphate and nitrogen sources on PHA production was determined by simply using carbon sources i.e. (starch, yeast, peptone, sucrose, maltose, glucose and date palm syrup), sugars were added at equivalent weights and the date palm syrup was used at different concentration ranged from 4% to 30% v/v. Also the effect of different concentration of potassium phosphate and ammonium chloride in range equivalent to 0.1 to 1% (v/v) were tested.

2.5 Extraction and Estimation of PHB Production Efficiency

PHB was extracted from the *Bacillus* by three methods, the first is the extraction by chloroform according to the methods of Hahn et al. [19] as follows, cells were collected by centrifugation at 4000 x g for 20 min at 25ºC, washed with acetone for 20 min. The dried cells were mixed with 50 volumes of chloroform for 48 h at 30°C. Centrifugation was used for recovery of PHB Finally, pure PHB was obtained by precipitation with a mixture of methanol and water (3:7 v/v) followed by filtration. Second method was the extraction using NaOH as strong base according to the method of Kunasundari and Sudesh [20]. Cells were collected by centrifugation at 4000 xg for 20 min at 25ºC and washed with water. The pelleted cells were dissolved in 0.2 N Na OH at 30ºC for 1 h. After one hour the cells were collected by centrifugation at 4000 xg and the pellet was washed by ethanol and acetone. The PHB was leaved in oven at 40ºC until it completely dried. Third method was extraction using sodium hypochlorite according to methods of Daniel et al. [21]. To about 0.2 g of lyophilized cell biomass, 5 ml Na OCl (12 %) was added and the mixture was leaved at 40ºC for 1 h. Subsequently, the PHB granules were collected by centrifugation (2000 xg). The pellet was then washed by water then by ethanol and acetone the insoluble residue was discarded and the pellet was dissolved in chloroform. The PHB granules were collected and weighed after evaporation of chloroform.

2.6 Quantifications of Bacterial Growth and Dry Weight

Cell growth was monitored by measuring the optical density (O.D) at 600 nm using spectrophotometer Ten milliliter culture medium was centrifuged at 10,000 rpm, 4ºC for 15 min and cell pellet was washed with 10 mL distilled water. Cell pellet was harvested by centrifugation and dried at 105ºC for 48 h [22] Cell mass concentration was determined by the standard calibration curve between OD 600 and cell dry weight.

PHA accumulation (%) = Dry weight of extracted PHA (g/L) / Cell dry weight (CDW) (g/L) × 100%

2.7 Quantification of PHA in Cell Suspensions

Standard PHA sample (0.02-0.1 g) was digested by heating in concentrated H_2SO_4 at 100ºC for 10 min estimated at 235 nm in UV/visible spectrophotometer to determine slope and easily calculate factor = 1/slope. By referring to the standard curve, the quantity of PHA produced was determined [23].

2.8 Identification of PHB Producing Isolate

Morphological and Biochemical Test

The characteristics of colony as its pigment, ability to hydrolyze starch, gelatin, casein and cellulose was detected. Also, the biochemical tests as indole production, methyl red, Vogues Proskauer, citrate utilization, motility, catalase were determined. The fermentation with sugar was also studied by spreading the isolate on medium containing different types of sugars (sucrose, galactose, glucose, fructose, sorbitol, xylose, mannose, rhaffinose, lactose, and ribose. The characteristics of the isolates were compared with the data from Bergey's Manual of Determinative Bacteriology [24].

2.9 Statistical Analysis

Statistical analysis was done using GraphPad InStat software. Results were expressed as mean ± SE. Statistical significance for data was determined using a one-way analysis of variance (ANOVA) with post-Dunnett test. The level of significance was accepted as $P < 0.05$.

3. RESULTS AND DISCUSSION

This research work is aimed to isolate and identify PHB producing bacteria by utilization of inexpensive alternate carbon sources native to Saudi Arabia such as date palm syrup. This target was achieved by screening of the bacterial isolates for their presence/absence of PHB using a Nile-red staining approach. The extracted PHB was analyzed and confirmed using IR spectra. Due to the high production cost of the PHB based on the use of multiple carbon sources, date palm syrup as alternative inexpensive substrates was used. By using a Nile-red staining assay, screening of the culture collection for presence/absence of PHB was performed. The bacterial isolate yielded positive results as indicated in (Fig 2). The results show that the isolate G-4 exhibited a very strong fluorescence in comparison to the negative controls, therefore recorded as PHB positive strains. The morphological and biochemical characteristics of G-4 were summarized as shown in Table 1.

Table 1. Morphological and biochemical characterization of the isolate G-4

Test	Reaction
Staining	Gram positive Bacilli
Spore staining	Spore forming bacteria
Biochemical properties	
Catalase test	Production of gas bubbles
Urease test	+
Indole formation	-
Methyl red test	-
Voges-Proskauer test	+
Citrate test	+
Growth in NaCl 7%	Grow
Growth at 10, 30 and 37°C	Grow
Hydrolysis of	
Casein	+
Cellulose	+
Starch	-
Carbohydrates fermentation	
Glucose	+
Sucrose	+
Fructose	+
Lactose	-
Xylose	+
Ribose	+

Preliminary identification indicated that G-4 isolate was Gram + Bacilli, spore forming bacteria, catalase positive, urease positive, indole formation negative, methyl red test positive, and Voges-Proskauer test negative, citrate test positive and formation of glucose, lactose, mannitol positive but without gasses in glucose and grow at 10, 30, 37°C and NaCl 7%. According to Bergey's Manual of Systematic Bacteriology, the isolate G-4 is most probably *Bacillus* sp. [24] which was also confirmed by the results obtained by Hassan et al. [25]. Some other studies reported that PHB can be isolated from microorganisms belonging to the genera *Azotobacter*, *Alcaligenes*, *Pseudomonas*, and *Bacillus* [26,27,28].

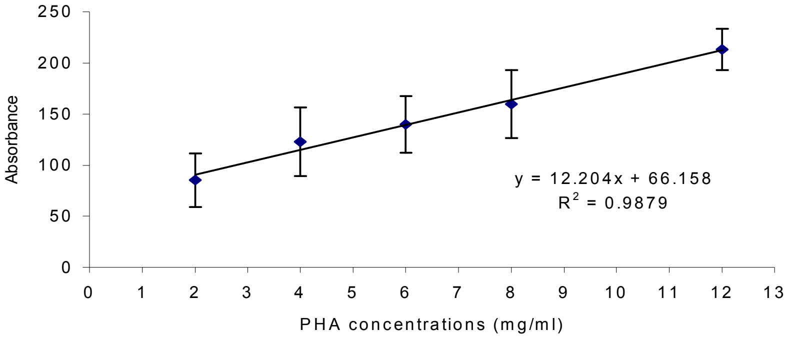

Fig. 1. Standard curve for PHA detection

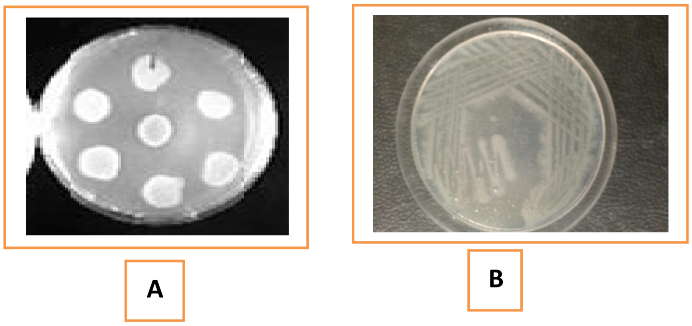

Fig. 2. Nile-red staining assay for presence/absence of PHB, (A) shows positive isolate & (B) negative isolate

To extract the PHB, various extraction methods either by chloroform, sodium hypochlorite and sodium hydroxide were performed. The results presented in Fig. (3) clearly show that the use of chloroform extraction method was time consuming and yielded low purity. On the other hand, the use of Na OH gave the best results compared to chloroform and sodium hypochlorite.

As shown in Fig (5) the absorption bands appeared in the spectrum are associated with the side chains from the ester C=O stretching vibration at 1727 cm^{-1}, the CH_3-deformation peak at 1286 cm^{-1} and the ester C-O-C at 1072 cm^{-1} which clearly put the extracted polymer sample obtained from isolate G-4 in the class of polyhydroxybutyric acid. Gurubasappa et al. [29] reported that, FTIR spectra of the extracted polymer show peaks at 1731.92 cm-1 and 1215.47 cm-1 corresponds to specific rotations around carbon atoms specific to certain functional groups. Another study carried out by Oliveira et al. [30] show the peak at 1731.92 cm-1 corresponds to C=O stretch of the ester group present in the molecular chain of highly ordered crystalline structure. While the study of Rohini et al. [31] reported, the peak at 1215.47 cm-1 corresponds to –CH group. These peaks are corresponding to the peaks obtained for the standard PHB, at 1730 cm-1 and 1216 cm-1 exactly confirming that the extracted polymer is PHB and the Fourier-transform infrared (FTIR) absorption band at about 1,730 cm-1 is a characteristic of the carbonyl group and that a band at about 1,280–1,053 cm-1 characterizes valance vibration of the carboxyl group.

To achieve enough biomass from isolate G-4 required as inoculum for PHB production, various growth media (LB, MSM and SG) and incubation times (24, 48 and 72 hr) at 30ºC were changed. As shown in Fig. 5, MSM medium yielded the highest cell biomass, which therefore used in the further studies and incubation time for 72 hours (Figs. 6 & 7).

The optimized (MSM) was prepared as previously described [17] and the medium was initially adjusted at different pH values ranged from 6.5 to 8.5. Under the optimized growth conditions (incubation at 37ºC for 48 hours in MSM medium, the effect of pH on the growth rate of isolate G-4 was examined. As shown in Fig. (8), the results revealed that the highest growth rate (O.D 600 =0.85) was observed at pH 7.2.

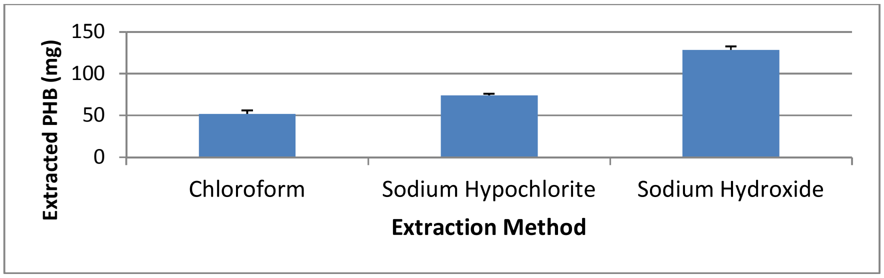

Fig. 3. PHB yields with using different extraction methods

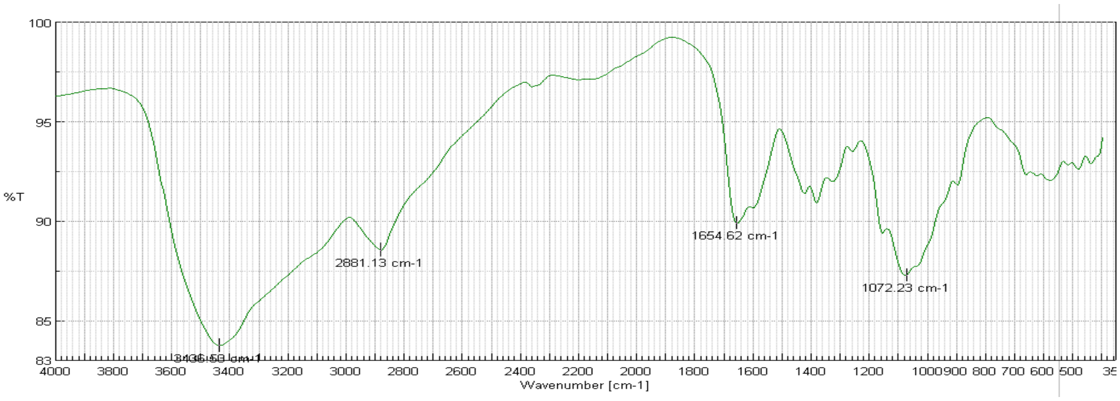

Fig. 4. IR spectrum of the standard PHB

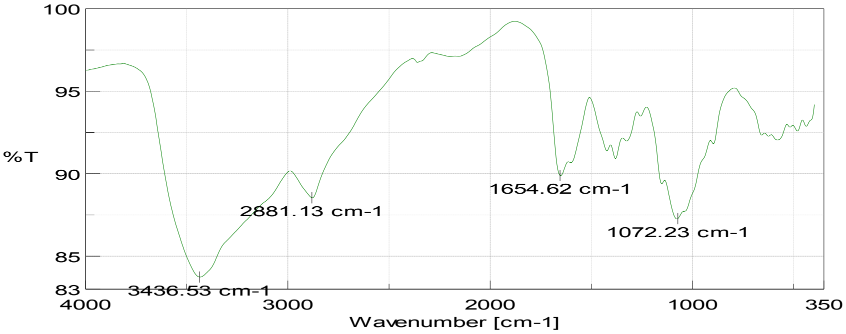

Fig. 5. IR spectrum of the extracted biopolymer from isolate G-4

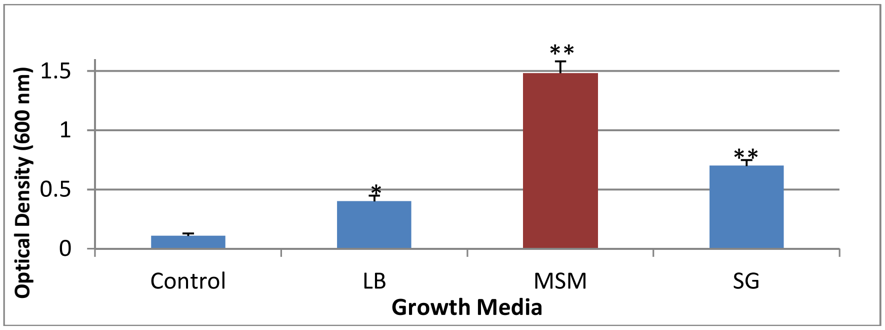

Fig. 6. Growth optimization of isolate G-4 on different nutrient media. Experiments were done in triplicate and data represented as an average ± standard deviation.

**= p<0.05; **= p<0.01*

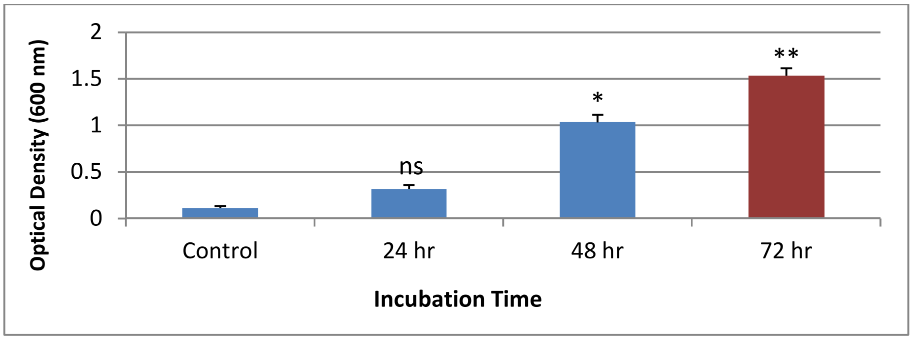

Fig. 7. Growth optimization of isolate G-4 on different incubation times. Experiments were done in triplicate and data represented as an average ± standard deviation.
*ns= Non significant; *= $p<0.05$; **= $p<0.01$*

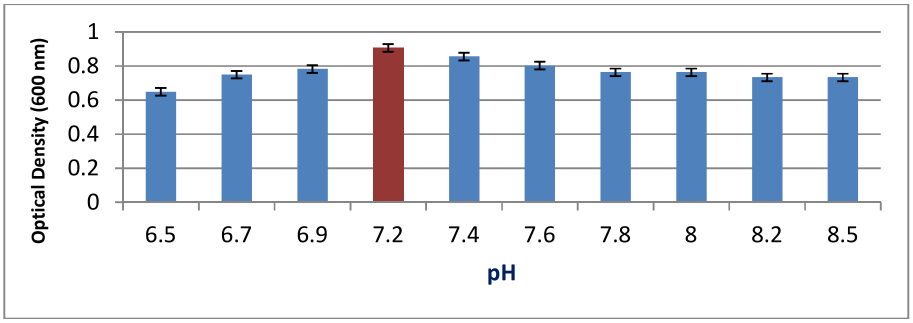

Fig. 8. The effect of different pH values on the growth of bacterial isolate G-4

Rukman et al. [32] investigated the Halomonas elongate can used as bioplastic producer. The indication as bioplastics PHB producer was evaluated by growing in Nile red-containing medium and bacterial colonies displayed bright orange fluorescent under ultraviolet light [33]. The effect of different carbon sources, nitrogen, and pH values on PHB production by strains of Rhizobium meliloti was investigated by Tavernler et al. [34] these strains showed higher PHB content at pH 7.0. These findings are in agreement previously reported studies [35]. These results supported by Sangkharak and Prasertsan [36]. Pozo et al. [11] studied effects of culture conditions on PHB production by *Azotobacter* sp. and showed that growth conditions including pH, temperature plays an important role in the production rate of PHB.

Under the optimized growth conditions, different concentrations of various carbon sources (2-40 g/l) were tested. The data presented in Fig. (9) show that the PHB yield was recorded as follows: glucose (10 g), mannose (5 g/l), maltose (9 g/l), lactose (10 g/l), sucrose (20 g/l), Yeast extract (15 g/l).

The strain P. hydrogenovora DSM 1749 has been reported to co-metabolize glucose and galactose from lactose-hydrolyzed whey permeate to produce PHB [37,38]. *Pseudomonas* cepacia ATCC 1775 produce high quantity of PHB at supplementation of culture media with lactose and xylose [39]. Nath et al. [40] reported the PHB production from lactose and sucrose supplementation by Methylobacterium sp. ZP24 and from bagasse as well as from food wastes [41].

The effect of different concentrations of date palm syrup (1-30%; v/v) as inexpensive carbon source in (MSM) with incubation time for 48 h at 37°C, were tested. The data revealed that the highest amount of PHB (5 mg/ml) produced by the isolate G-4 was achieved with date palm syrup at concentration of 8% (Fig. 10).

Page, [42] reported that instead of glucose, molasses, the byproduct in sugarcane industry can be used as a carbon source for PHB production by *Azotobacter vinelandii.*

The effect of phosphate (KH_2PO_4) and ammonium (NH_4Cl) on the PHB production was examined. Isolate G-4 was grown under the above optimized growth conditions in (MSM) containing various concentrations of ammonium and phosphate ranged from 0.1-1% (w/v). As shown in (Figs. 11 & 12), it was observed that the concentrations of phosphate (0.04%) and ammonium (0.2%) gave the highest PHB yield.

The results of this study were agreement with those obtained by Shaaban et al. [43] Khanna and Srivastav [44], who reported the high content of PHB production at using MSM medium supplemented with ammonium sulphate by R. *eutropha*, *Stenotrophomonas* sp. and *Pseudomonas* sp. As well as Raje and Srivastav, [45] reported PHB accumulated by A. *eutrophus* with different supplementation of the culture media with ammonium salts.

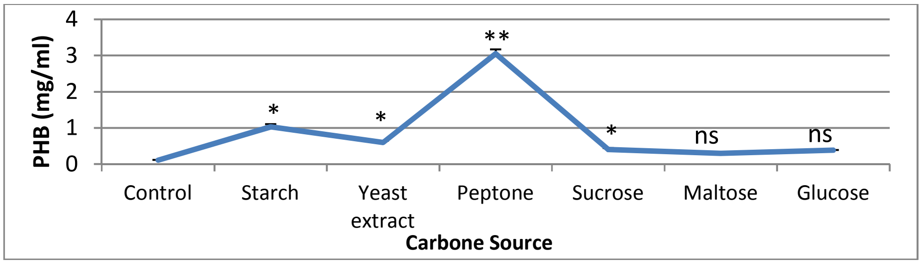

Fig. 9. The effect of different carbon sources on PHB content. Experiments were done in triplicate and data represented as an average ± standard deviation.
*ns=Non significant; *= p<0.05; **= p<0.01*

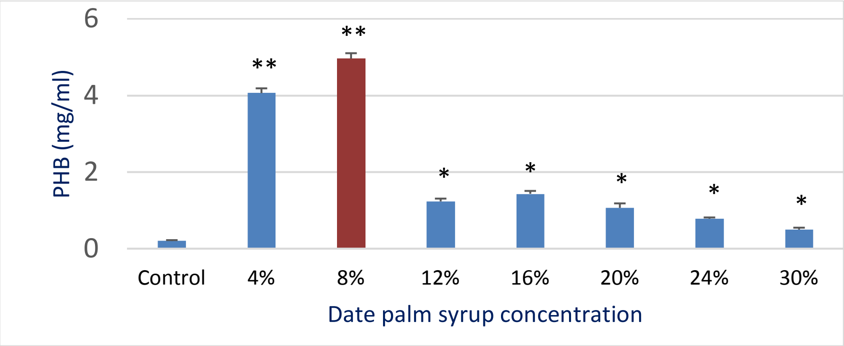

Fig. 10. The effect of different date palm syrup concentrations on the production of PHB. Experiments were done in triplicate and data represented as an average ± standard deviation.
**= p<0.05; **= p<0.01*

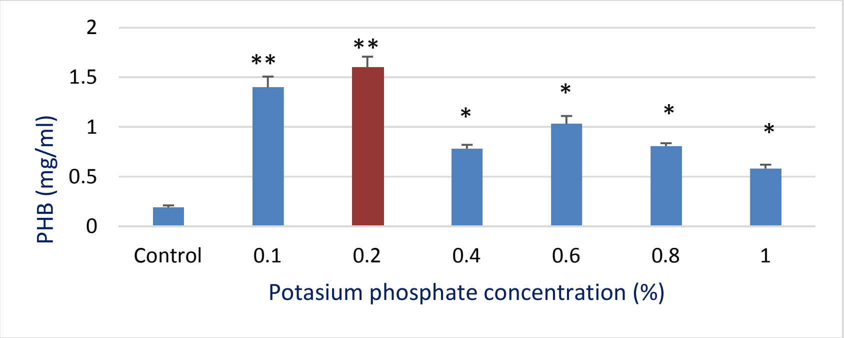

Fig. 11. The effect of different Phosphate concentrations on the production of PHB. Experiments were done in triplicate and data represented as an average ± standard deviation.
**= p<0.05; **= p<0.01*

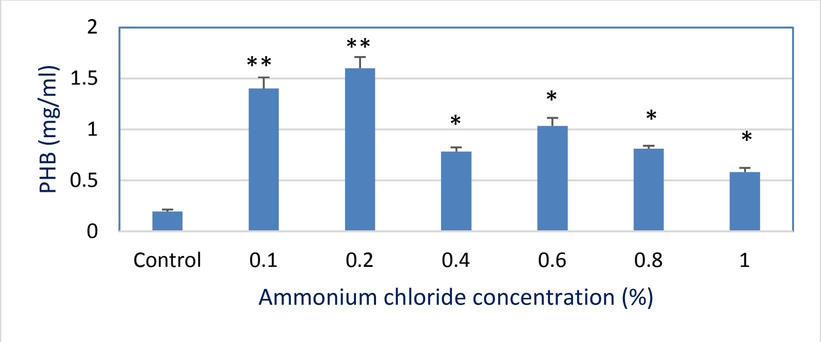

Fig. 12. The effect of different Ammonium concentrations on the production of PHB. Experiments were done in triplicate and data represented as an average ± standard deviation.
**= p<0.05; **= p<0.01*

4. CONCLUSION

These results show that *Bacillus* species identified in soil sample of Al-Kharj produced highest concentration of PHB by using date palm syrup as a carbon source that can substantially reduce substrate and production costs of PHB.

CONSENT

It is not applicable.

ETHICAL APPROVAL

It is not applicable.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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Peer-review history:
The peer review history for this paper can be accessed here:
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RASĀYAN *J. Chem.*
Vol. 10 | No. 1 |124-135 | January - March | 2017
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

ASSESSMENT OF HEAVY METALS IN GREEN VEGETABLES AND CEREALS COLLECTED FROM JAMKHANDI LOCAL MARKET, BAGALKOT, INDIA.

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ABSTRACT

Heavy metals determination in Cereals and vegetables is of vital interest because of their essential or toxic nature. In order to assess the levels and impact of different trace metals on human health, a study was carried out to determine the levels of different trace heavy metals present in commonly edible cereals and vegetables which are available in the local market of Jamkhandi City. Industrial effluents, domestic waste, municipal sewage water, agricultural runoff -significantly affected the water quality on short- and long –term basis. The present investigation reveals with the assessment of heavy metals in soils, selected cereals and green vegetables available in the region irrigated with contaminated water. All the samples were analyzed using Flame photometer (Elico), Atomic Absorption Spectrophotometer (Elico). The concentrations of most of the heavy metals were found in the normal legal limit in irrigation water, soil samples and food set as compared with international regulations. The obtained results declared that concentrations of metals were exceeding than the recommended maximum acceptable levels. The concentration of heavy metals in wheat gains of lands was found to be in the order of Cu>Zn<Ni<Cd. Other grains and green vegetables were analyzed for heavy metals such as Mn, Pb, and Fe, all were beyond recommended dietary limits. It is recommended that treatment facility must be installed to reduce heavy metals concentrations of waste water being used for downstream irrigation. The study suggests that contaminated water irrigation led to the accumulation of heavy metals in foodstuff causing potential health problems for consumers.

Keywords: Heavy metals, Cereals, Green vegetables, Municipal wastewater and industrial effluents.

INTRODUCTION

Heavy metal contamination in cereals and vegetables cannot be underestimated as these foodstuffs are important components of the human diet. The cereals most commonly cultivated in this region are wheat, Jawar, Barley, Sorghum, Rice, Sajji etc. These cereals are the important as well as very nutrient grains. Also is more stable food for most people of the area. Cereals are needed for a healthy diet because cereals derived products are recommended due to their contents such as fiber, trace minerals, and vitamins, which support to prevent various diseases. But, Heavy metals contamination in food products more than tolerance limit leads adverse effect on health. The cereals are rich in carbohydrates, protein etc., and act as sources of energy. Therefore, they are essential and useful for a well-balanced healthy diet. Vegetables are rich sources of vitamins, minerals, and fibers, and also have beneficial antioxidative effects. However, intake of heavy metal-contaminated vegetables may pose a risk and pose a direct threat to the human health. Heavy metal contamination of the food items is one of the most important aspects of food quality assurance[1,2].

Food safety and potential health risks

Rapid and unorganized urban and industrial developments have contributed to the elevated levels of heavy metals in the urban environment of developing countries such as Egypt[3], Iran[4], China[5]and India[6]. In urban and peri-urban areas, land contamination with toxic metals is common as a result of the industrial and municipal activity. Wastewater irrigation to increase the yield of food crops (vegetables) is the

Rasayan J. Chem., 10(1), 124-135 (2017)
http://dx.doi.org/10.7324/RJC.2017.1011575

principal source of contamination in urban agricultural lands[7]. These effluents are rich in toxic metals and are a chief contributor to metals loading in waste irrigated and amended soils[8,9]. Emissions of heavy metals from the industries and vehicles may be deposited on the vegetable surfaces during their production, transport and marketing. Recently, have reported that atmospheric deposition can significantly elevate the levels of heavy metals contamination in vegetables commonly sold in the markets of Varanasi[6], India.

Heavy metals are among the major contaminants of food and may be a major problem to environment[3,10]. The heavy metals may enter the human body through consumption of contaminated drinking water, consumption of food plants, cereals and green vegetables grown in the metal contaminated soil and sediments[10]. Heavy metals are potential environmental contaminants of causing human health problems if present in a higher percentage of the food grains. The heavy metals showed toxic effects even at very low concentration[11]. Heavy metals are non-biodegradable and persistent, have long biological half-lives and they can be bioaccumulated through the biological chains. Soil – plants, green vegetables and food leading to unwanted side effects. The high amount of heavy metals in environment represents a potential danger to human health due to their extreme toxicity. Heavy metal contamination may be occurred due to the irrigation with contaminated water from municipal wastes, industrial effluents, the addition of inorganic fertilizers, metal based pesticides and agricultural practices. Crops and green vegetables grown in soils contaminated with heavy metals have a greater accumulation of heavy metals than those grown in uncontaminated soil[12].Many researchers emphasized the toxic effects of heavy metals to the human body. The elements such as Cd, Cr and Arsenic are considered as carcinogenic (cancer producing elements), while Fe, Cu, Zn, Ni and Mn are considered as essential elements. But, these elements are found in higher than their permissible limits may create a toxic effect in human[13,14].

Metal Toxicity and Health Risk

Lead toxicity in the body can cause – musculoskeletal, renal, ocular, immunological, neurological, reproductive and developmental effects. Cadmium intake is known to result in bone fracture, cancer, diarrhea, stomach pains, severe vomiting, reproductive failure and damage to thecentral nervous system. In addition to this cardiovascular, kidney, nervous as well as bone disease[15,16]. Heavy metals have also been implicated in causing carcinogenesis, mutagenesis and tetra genesis[17]. A complete profile of heavy metals in foodstuffswas not published so far. Thus, the aim of this study was therefore to evaluate and compare the concentrations of heavy metals in cereals available in the local markets for the consumers in Jamkhandi city and causing health hazardous with the consumption of these cereals.

Vegetables are of great importance in the diet because of the presence of vitamins and mineral salts. In addition to this green vegetables contain water, calcium, iron, sulfur and potash[18]. Vegetables are very important protective food and useful for the maintenance of health and the prevention and treatment of various diseases[19]. The elements like Cd, Pb, and Hg will cause a major problem to our environment while the elements like Cu, Zn, Fe, Sulphur and Mn are essential for biochemical reactions in the body[20]. Generally, most of the heavy metals are not biodegradable, have long biological half-lives and have the potential for accumulation in the different body organs leading to unwanted side effects[16].

The toxicity of metal ions is correlated to one another; the Copper toxicity induces iron deficiency, lipid peroxidation and destruction of membranes[20]. High level of Nickel may result in Zinc or Iron deficiency as well as enzymic malfunctioning[16].Based on persistent nature, accumulation behavior and the probability of potential toxicity effects of heavy metals as a result of consumption of green vegetables and food grains. Hence, there is need to assess trace elements present in food grains and green vegetables and some recommendations were made to human diet.

Study Area

The study was conducted on food grains, vegetables from the local market of Jamkhandi city (taluk place of Bagalkot district) river water quality, soil properties were investigated from the four villages of Jamkhandi taluk viz; Hipparagi, Surapali, Savalagi and Hire Padasalagi, all these villages are located on or along the Krishna river belt. The cereals and vegetables are exporting daily or seasonally to the Jamkhandi marketplaces.

EXPERIMENTAL

Materials and Methods

All the reagents used for analytical grade highly purified de-ionized double distilled water (DDW) was used for dilution and preparation of reagents and working standards. All glass wares, plastic wares used, were thoroughly washed with liquid soap, rinsed with distilled water, soaked in 10% nitric acid for 24 hours, once again cleaned thoroughly with DDW and dried in such a manner to ensure that any contamination does not occur. All collected samples were stored in clean polyethylene bags, and used for analyses.

Sampling and sample preparation

For soil sampling, four random bowls of cereal fields were selected (Hipparagi- spot S1, Surapali-Spot S2,Savalagi-spot S3 and Hire Padasalagi-spot S4) at a mutual distance of about 20 feet were collected from the surface, at the same period water samples were collected to know their Physico-chemical parameters. The soil samples were oven dried overnight at 80 – 90ºC, gently ground and sieved to 2 mm mesh size, homogenized, and used for heavy metal and other parameters analysis. At harvest time, cereal samples were collected from each field and washed with DDW to remove the adhered soil, dust and other contaminants. The selected cereals were oven dried for 48 hours at 70ºC and then ground to pass a 1 mm sieve for determination of heavy metal contents.

A total of six samples of vegetable were purchased from the central place of Jamkhandi city during 2016.The collected samples were washed with distilled water to remove the dust particles. Then samples were cut into small pieces using a clean knife. Edible portions of the samples were used for analysis; the leafy vegetables included Spinach (Palak), Fenugreek (Methi), Radish(Mulangi),Deccan hemp(Pundi), Coriander (Kotambari) and Dill(Sabasagi).All the samples were collected and stored in polyethene bags until analysis under refrigeration condition (<10ºC). The samples for analysis were then dried using the oven dry method at 105ºC for 24 hours (AOAC, 1990), and a mixture grinder was used to powder the samples while preventing oven heating.

About 1 g of the samples were weighed and digested in a mixture of 5 ml of HCl, 2 ml of Conc H_2SO_4 and 20 ml of Conc. HNO_3 in a conical flask under a fume hood. The content was mixed and heated gently at 180ºC – 220ºC for about 30 min on a hot plate. The content was heated until dense white fumes appear. It was then heated strongly for about 30 min then allowed cooling before making up to the mark in 50 ml volumetric flask. This digested solution used to determine the micro-nutrients like Cadmium (Cd), Chromium (Cr), Cobalt (Co), Copper (Cu), Iron (Fe), Lead (Pb), Manganese (Mn), Nickel (Ni) and Zinc (Zn)by using Atomic Absorption Spectrophotometer (Elico). The instrument setting and operational conditions were done in accordance with the manufacturers' specifications.

Plant samples and food grains used for analyses

Edible part of vegetable / cereal	Common name	Botanical name	Family
Leaf	Spinach (Palak)	Beta vulgaris L.	Chenopodiaceae
Leaf	Fenugreek (Methi)	Trigonella foenum-graecum	Legumes
Stem	Radis (Mulangi)	Raphanus sativus L.	Brassicaceae
Leaf	Deccan hemp(Pundi)	Hibiscus cannabinus	Malvaceae
Leaf	Coriander (Kotambari)	Coriandrum sativum	Umbelifers
Leaf and stem	Dill (Sabasagi)	Anethum graveolens	Apiaceae
Grain	Wheat	Triticum	Poaceae
Grain	Jowar (Pure)	Sorghum bicolor	---
Grain	Jowar (Medium)	---	---
Grain	Sajji	---	---

Table-1: Water quality parameters of selected spots and comparison with standards WHO, ISI, BIS. [S1-Hipparagi, S2-Surapali, S3-Savalagi and S4-Hirepadasalagi, Villages]

S. No.	Parameters	S_1	S_2	S_3	S_4	Average	WHO	ISI/BIS
1	Temperature	22	21	20	18	20	---	---

2	pH	7.5	7.6	7.8	7.2	7.5	6.5-7.8	6.5-8.5
3	EC	3470	1913	1827	1648	1652	400	1400
4	TA	42.2	46.1	48.9	50.2	46.9	120	200-600
5	TH	48.5	52.6	49.2	40.5	47.7	300	300
6	Na^+	32.5	31.2	38.5	40.2	35.6	200	200
7	K^+	10.2	8.9	9.2	10.0	9.6	1.4	1.4
8	DO	6.5	6.6	6.6	6.6	6.6	7	7
9	NO_3	45.3	41.2	40.5	38.5	52.7	40-100	40-100
10	Cl^-	48.6	42.5	40.4	39.5	42.8	250-1000	250
11	SO_4	42.5	39.2	49.2	36.9	41.95	150-250	150-200
12	Cr	0.1	0.1	0.1	ND	0.1	0.05	0.05
13	Cu	0.5	0.4	0.5	0.5	0.5	2.00	2.00
14	Fe	1.16	1.14	1.12	1.10	1.13	<1	0.3
15	Ni	0.05	0.06	0.06	0.05	0.06	0.02	0.02
16	Cd	0.03	0.02	0.02	0.03	0.03	0.01	0.01
17	Pb	0.25	0.22	0.23	0.19	0.22	0.05	0.05
18	Zn	7.2	7.6	6.8	7.0	7.2	5	5
19	Mn	0.5	0.5	0.6	ND	0.5	>0.5	0.3
20	Ca	36.2	42.8	45.9	50.2	43.8	75-100	75-100
21	TDS	1613	1012	931	856	1103	<500	500

Table-2: Physico-chemical parameters and other nutrients in soil samples of selected four locations (mg/kg dried weight basis)[S1-Hipparagi and S2-Surapali, S3-Savalagi and S4-Hirepadasalagi, Villages]

S.No.	Parameter	UNIT	Spot S_1	Spot S_2	Spot S_3	Spot S_4	Legal limit
I	Physical-Parameters						
	Bulk Density	g/cc	1.14	1.11	1.11	1.12	
	Water Holding Capacity	%	56	57	57	57	
	Texture		Black	Black	Black	Black	
II	Chemical Parameters						
	pH		8.04	7.71	7.90	8.25	6.5-7.5
	EC	ds/m	1.16	1.05	1.01	4.56	<1
	Sodium	%	0.51	0.62	0.25	0.84	<0.1
	Calcium Carbonate		Medium	Medium	Medium	Medium	
III	Major Nutrients						
	Organic Carbon	%	1.08	0.98	2.08	0.95	0.5-0.75
	Available N	Kg/h	310.2	269.3	278.6	259.3	250-280
	Total N	%	0.102	0.112	0.110	0.042	0.03-0.06
	Available P	Kg/h	43.6	76.2	28.9	66.8	20-60
	Available K	Kg/h	284	235	248	365.3	250-300
IV	Secondary Nutrients						
	Ca	%	22.5	18.3	14.8	22.8	<1
	Mg	%	9.23	3.10	3.50	0.26	<0.5
	SO4	ppm	18.6	5.12	12.3	17.3	10-20
V	Micro Nutrients						
	Iron (Fe)	ppm	4.51	4.41	3.41	3.21	Min.4.50
	Manganese	ppm	2.94	3.12	1.91	1.3	Min.2.00
	Zinc (Zn)	ppm	0.95	0.87	0.72	0.68	Min.0.75
	Copper (Cu)	ppm	1.33	0.63	0.91	0.82	Min.0.60
	Cadmium	ppm	0.54	0.36	0.28	0.17	Min. 0.2
	Chromium	ppm	1.18	1.06	0.89	0.80	Min. 0.02
	Lead	ppm	0.10	0.09	0.08	0.10	0.05-0.2

	Nickel	ppm	1.31	0.24	0.53	0.88	Min. 0.50
	Boron	ppm	0.95	0.68	0.78	0.88	Min.0.50
	Molybdenum	ppm	0.11	0.10	0.09	0.08	0.05-0.2

Table-3: Concentration of Heavy Metals (ppm dry weight) in Cereal Samples ofselected Lands.

Metal (ppm)	Wheat	Jawar (Pure)	Jawar (Medium)	Sajji	Tolerance limit(ppm)	WHO Safe limit
Cultivation lands of Hire Padasalagi village.						
Copper	3.15	1.70	2.45	2.18	3	---
Iron	38.83	23.00	32.05	21.45	20	---
Zinc	333.75	195.50	172.25	232.25	27.4	---
Manganese	51.25	10.75	16.38	13.65	2	500
Cobalt	0.14	0.11	0.13	0.15	---	50
Nickel	0.08	0.18	1.40	1.00	1.63	67
Chromium	0.22	0.20	0.18	0.15	0.02	2.3
Lead	0.09	0.08	0.065	0.054	0.2	0.3
Cadmium	ND	ND	ND	ND	0.2	0.2
Cultivation lands of Savalagi village.						
Copper	3.28	2.78	2.59	2.80	3	---
Iron	38.92	24.2	35.2	22.08	20	---
Zinc	341.12	197.51	173.98	233.10	27.4	---
Manganese	52.38	11.21	17.31	14.12	2	500
Cobalt	0.24	0.18	0.12	0.25	---	50
Nickel	0.09	0.19	1.48	0.92	1.63	67
Chromium	0.49	0.31	0.29	0.19	0.02	2.3
Lead	0.110	0.100	0.072	0.061	0.2	0.3
Cadmium	ND	ND	ND	ND	0.2	0.2
Cultivation lands of Hipparagi village.						
Copper	4.15	3.75	3.82	3.54	3	---
Iron	39.9	25.9	38.91	26.2	20	---
Zinc	353.81	201.10	181.21	239.12	27.4	---
Manganese	55.40	13.92	19.12	17.21	2	500
Cobalt	0.49	0.39	0.13	0.46	---	50
Nickel	0.11	0.25	1.55	1.08	1.63	67
Chromium	0.85	0.42	0.331	0.19	0.02	2.3
Lead	0.163	0.130	0.09	0.08	0.2	0.3
Cadmium	ND	ND	ND	Nd	0.2	0.2
Cultivation lands of Surapali village.						
Copper	3.98	3.01	3.12	3.12	3	---
Iron	39.1	24.9	36.2	24.5	20	---
Zinc	348.20	198.15	174.52	234.25	27.4	---
Manganese	53.92	12.91	17.98	15.20	2	500
Cobalt	0.35	0.25	0.12	0.34	---	50
Nickel	0.10	0.23	1.50	1.01	1.63	67
Chromium	0.68	0.49	0.39	0.21	0.02	2.3
Lead	0.141	0.110	0.08	0.07	0.2	0.3
Cadmium	ND	ND	ND	ND	0.2	0.2

RESULTS AND DISCUSSION

The contaminated water used for irrigation was analyzed for temperature, turbidity, DO, pH, EC, TDS, TA, TH, Carbonates, bicarbonates, chloride, sulphate, calcium and heavy metals were reported in table 1. The results revealed that TDS, EC, K, Ni, Cd, Pb, Zn and Fe were found higher than the permissible limits given by the National Standards for drinking water quality.

From the findings and by the fact that the soil at these sites contaminated with heavy metals found above permissible limits. The sites of Hipparagi and Surapali have been irrigated with polluted waste water (municipal sewage water) from Rabakavi and Banahatti industrialized and urbanized towns. Hence, the most prevalent heavy metals such as Fe, Mn, Zn, Cu, Cd and Cr in the soil samples found to be in higher concentrations as reported in Table 2.

Table 3 reports the results of heavy metals in wheat grains, Jawar (pure), Jawar (Medium) and Sajji from the cultivated lands of Hipparagi, Surapali, Savalagi and Hire Padasalagi villages, where the crops were irrigated with River Krishna amendments with municipal sewage waste, solid waste etc.,

Heavy Metal Concentrations in Cereals

Copper (Cu)

Copper is one of the essential micronutrients in plants and animals[21]. The human body contains Cu at a level of 1.4 to 2.1 ppm of body mass. Cu is absorbed in the intestine (gut), which facilitates iron uptake. Its deficiency can produce anemia- like symptoms, neutropenia, bone abnormalities, increased incidence of infections, and abnormalities in glucose and cholesterol metabolism. In the present investigation the concentration of Cu in the wheat grains was found to be in the range of 3.15 ppm to 4.15 ppm from all selected cultivated lands, the values were found higher than the tolerance limit, this is the indication that the soils of the region received a high metal load through the application of contaminated sewage water, solid wastes etc., the order of Copper concentration in wheat grains as compared with other cereals like Jawar (Pure), Jawar (Medium) and Sajji was as: Wheat > Jawar (Medium) > Jawar (Pure) > Sajji. From the investigation, it is revealed that the Copper concentration in wheat grains found more than other cereals.

Iron (Fe)

Iron is an essential element in man and plays a vital role in the formation of hemoglobin, oxygen and electron transport in human body[22]**.** In the present investigation, Iron was found to have the highest concentration in the entire cereals samples analyzed (table 3). The maximum concentration of iron was found in wheat (39.9 ppm) at Hipparagi cultivated irrigated lands. The tolerance limit of Iron in food is found to be 20 ppm. The results obtained in this study were higher than the recommended limit. The total accumulation of Fe was in the order of Wheat > Jawar (Medium) > Sajji > Jawar (Pure). Hence, the study revealed that there was a significant difference in levels of Fe in the cereals.

Zinc (Zn)

Like Copper, Zinc is a most studied element in wheat grains, it is essential to all organisms and has an important role in metabolism, growth etc., Zn deficiency leads to coronary heart diseases and various metabolic disorders[23]. In the current study, the values of Zn was found to be in between 353.81 ppm – 333.75 ppm. The highest value found in the wheat grains of Hipparagi cultivated lands, the lowest values found in the lands of Hire Padasalagi. The levels of Zn in other grains such as Jawar (Pure), Jawar (Medium) and Sajji were found to be 201.10 ppm, 181.21 ppm and 239.12 ppm respectively from cultivated lands of Hipparagi locations; all values were higher than the prescribed range. It was evident from table 2 that deposition of heavy metal in soils by the uses of municipal waste water, sewage sludge etc., The content of Zinc reported in this investigation is generally higher than the permissible levels in all selected cultivated lands set by sttandards[24]. The study revealed that there was significant deference 5 ppm to 7 ppm in levels of Zinc in all cereals.

Manganese (Mn)

Essential for many biochemical processes. Kidney and liver are the main storage places for the Mn in the body, Mn is essential for the normal bone structure, reproduction and Mn play very important role in the functioning of the central nervous system. The deficiency of Mn causes reproductivity failure in both male and female[23]**.** Mn found in maximum concentration in wheat at Hipparagi cultivated lands (55.40 ppm) and minimum in Jawar (Pure) (13.92 ppm) in the same area the concentration of Mn in the cereals were found in the order: Jawar (Pure) < Sajji < Jawar (Medium) < Wheat; as reported in Table-3.

Cobalt (Co)

Cobalt is an important component of the vitamin B-12 molecule. It is required in the manufacture of RBC and in preventing anemia. An excessive intake of Cobalt may cause the over productionof RBC[22]**.** In the current study the maximum concentration of Cobalt found in wheat (0.49 ppm) of Hipparagi cultivated lands and minimum value of Cobalt found (0.13 ppm) in Jawar (Medium) of the same locations – the concentration of Cobalt in cereals samples were found in the order of Wheat > Sajji > Jawar (Pure) > Jawar (Medium) respectively (Table 3). The same trends were seen in other selected region of irrigated lands.

Nickel (Ni)

Enzymes functions are purely depended on the presence of Nickel. The trace amounts of Ni may be beneficial to activate somebody systems, but its toxicity at higher levels is more enzyme prominent[25]**.** The present findings of Ni in selected cereals found in between 1.55 ppm to 0.08 ppm which is less than the tolerance limit in cereals (1.6 ppm). Ni in wheat grain is 0.11 ppm, which is under the permissible limit. The order of Ni levels in Hipparagi cultivated lands were recorded as: Jawar (Medium) > Sajji > Jawar (Pure) > Wheat.

Chromium (Cr)

Chromium is an essential element required for normal sugar and fat metabolism even though chromium has been classified as not essential for mammals[26]**.** It is effective to the management of diabetes and it is a cofactor with insulin. Cr (III) and its derived compounds are not considered a health hazard, while the toxicity and carcinogenic properties of Cr (VI) have been known for a long time[27]**.** The concentration level of Cr in Hipparagi cultivation lands in wheat, Jawar (Pure), Jawar (Medium) and Sajji were found to be 0.85, 0.42 0.33 and 0.19 ppm respectively. These values are lower than the maximum permissible limit of 2.3 ppm by FAO/WHO[24]**.** The Cr content in wheat grains was found to be higher in almost all cases of selected cultivated lands as reported in table 3.

Lead (Pb)

Lead toxicity is known to cause muscular, skeletal, neurological, reproductive and developmental effects[28]**.** Higher concentrations of Lead reduce the growth, biomass and total chlorophyll content of plants. Consumption of cereals containing higher concentrations of Lead in the form diet may increase blood Pb levels with increases risk of anemia and neurological disorders. It is concluded that the increment of total solid heavy metals contents (Cd, Pb, Zn, and Cu) could enhance gains Cd accumulation and the increment of total soil Zn content may lower Pb accumulation in grains.

The current study reveals that the higher value of Lead in wheat grains (0.163 ppm) of Hipparagi cultivation lands and ranging from 0.163 ppm to 0.08 ppm in all grains, this is the indication that the cultivated soils were irrigated by waste water or amended by sludge in the region of Hipparagi, the other three selected villages such as Surapali, Savalagi and Hire Padasalagi are away from the dumping spots of municipal sewage of Rabakavi and Banahatti towns into the River Krishna downstream.

Cadmium (Cd)

Cadmium is highly toxic non-essential heavy metal and it does not have a role in the biological process in living organisms. Even lower concentration of Cd in the food chain could be harmful to living organisms[28]**.** Cd poisoning in man could lead to anemia, renal damage, bone disorder and concern of lungs (Edward et al ., 2013). Cadmium usually added to the soil by the uses of phosphatic fertilizers and industrial wastes may have a detrimental effect on soil micro-organisms. On the analysis of soil samples of the study area the concentration of Cd metal found to be 1.18 ppm, 1.06 ppm, 0.89 ppm and 0.80 ppm in Hipparagi, Surapali, Savalagi and Hire Padasalagi cultivation lands respectively. As can be seen from the current study (table 3) Cd was not detected in any of the cereal samples in the study area.

Heavy Metals in vegetables

The heavy metal levels determined were based on plants dry weight. Levels of Cu, Zn, Ni and Mn were observed to be lowest in selected all vegetable samples, while the levels of Fe, Cd and Pb were the highest. Heavy metals affect the nutritive values of agricultural materials and also have a deleterious effect on human beings. The results of the vegetable analysis showed that the level of Pb in all samples was in between 30.5 ppm to 58.1 ppm. The Pb levels in vegetables were observed in the order of Sabasagi > Palak >Kotambari>Pundi> Mulangi > Menthe.

Cadmium (Cd)

A non-essential element in all the samples analyzed, its level was observed varying in between 6.1 ppm to 31.6 ppm. The order of Cd metal concentration in the selected green vegetables: Palak (31.6 ppm) >Pundi (14.5 ppm) >Kotambari (12.4 ppm) > Menthe (6.7 ppm) >Mulangi (6.3 ppm) > Sabasagi (6.1ppm). All values found above the tolerance limit, definitely will cause a hazardous effect on human beings.

Copper (Cu)

Copper is an essential micro- nutrient which functions as biocatalysts, required for body pigmentation in addition to Fe. Cu maintains a healthy central nervous system if it is within tolerance limits. It prevents anemia and interrelated with the function of Zn and Fe in the body. In the current study the concentration of Cu in all the tested vegetable samples varied between 19.5 ppm in Sabasagi to 45.2 ppm in Mulangi. Cu levels in other green vegetables found to be as Palak (23.5 ppm), Menthe (44.5 ppm), Pundi (24.2 ppm) and Kotambari (25.7 ppm) all values were within the prescribed legal limits.

Zinc (Zn)

One of the most important metals for normal growth and development in a human being is Zinc[29]**.** Its deficiency may be due to inadequate dietary intake. The concentration of Zn in the samples reported in this study varied between 58.9 ppm lowest in Sabasagi and 116.4 ppm highest in Mulangi. Concentrations of Zn metal in other vegetables were found to be as: Palak (75.5 ppm), Menthe (73.0 ppm), Pundi (64.2 ppm) and Kotambari (69.0 ppm).

Table-4:Concentration of Heavy Metals in Green Vegetables (ppm values) available in Local Market Places.

S. No.	Vegetable	Cu	Zn	Ni	Mn	Fe	Pb	Cd
1	Palak (Spinach)	23.5	75.5	12.7	174.0	1120.0	51.4	31.6
2	Menthe (Trigonella)	44.5	73.0	23.0	93.0	470.0	30.5	6.7
3	Mulangi (Radish)	45.2	116.4	13.8	51.2	841.7	34.6	6.3
4	Pundi (Deccan henp)	24.2	64.2	16.4	46.4	541.8	41.4	14.5
5	Kotambari (Coriander)	25.7	69.0	11.8	162.0	424.5	49.5	12.4
6	Sabasagi (Dill)	19.5	58.9	13.6	39.9	421.0	58.1	6.1
WHO Safe limit		50	300	50	300	270	10	3

Nickel (Ni)

Nickel plays some role in body functions including enzymes functions. It occurs naturally more in plants than in the animal flesh. It activates some enzymes systems in trace amount but its toxicity at higher levels in more prominent. The Ni levels in the samples tested varied between 11.8 ppm and 23.0 ppm with the lowest level observed in Kotambari (11.8 ppm) and highest observed in Menthe (23.0 ppm).

Manganese (Mn)

Manganese has little direct activity on its own in the body as it is an integral component of Vitamin B_{12}. The activity and its uses to the body system are similar to that of Vitamin B12. However, in this study its level varied between 39.9 ppm lowest in Sabasagi and 174.0 ppm highest in Palak. Menthe (93.0 ppm), Mulangi (51.2 ppm), Pundi (46.4 ppm) and Kotambari (162.0 ppm). The metal ion found within the safe limit in all the green vegetables.

Iron (Fe)

Iron metal concentration in selected all vegetable samples found more than the tolerance and safe legal limit. Its concentration found highest in Palak (1120.0 ppm) and lowest in Sabasagi (421.0 ppm). The order of the Fe in all vegetables were recorded as: Palak (1120.0 ppm) >Mulangi (841.7 ppm) >Pundi (541.8 ppm) >Menthe (470.0 ppm) >Kotambari (424.5 ppm) > Sabasagi (421.0 ppm).

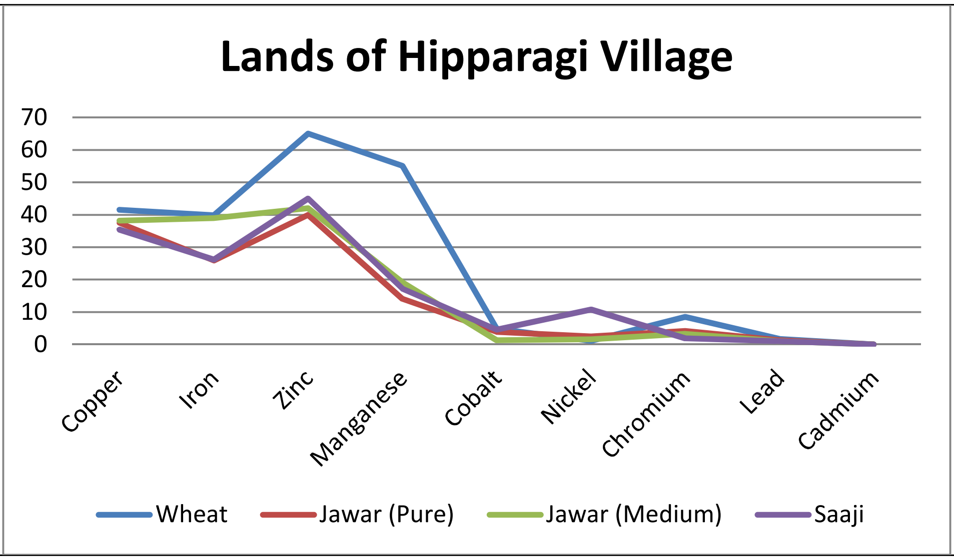

Fig.-1.Heavy Metals (ppm dry weight) in Cereals samples of Lands of Hipparagi Village.

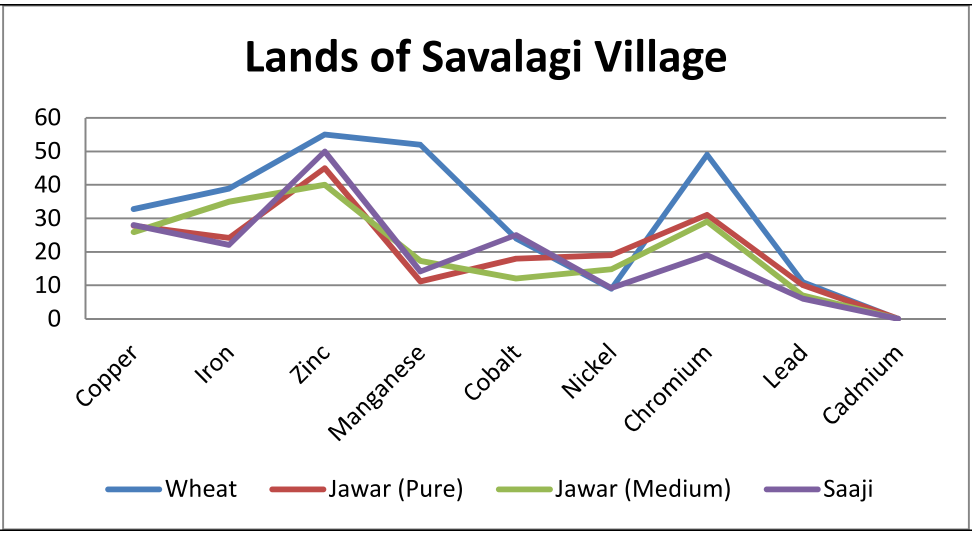

Fig.-2. Heavy Metals (ppm dry weight) in Cereals samples of Lands of Savalagi Village.

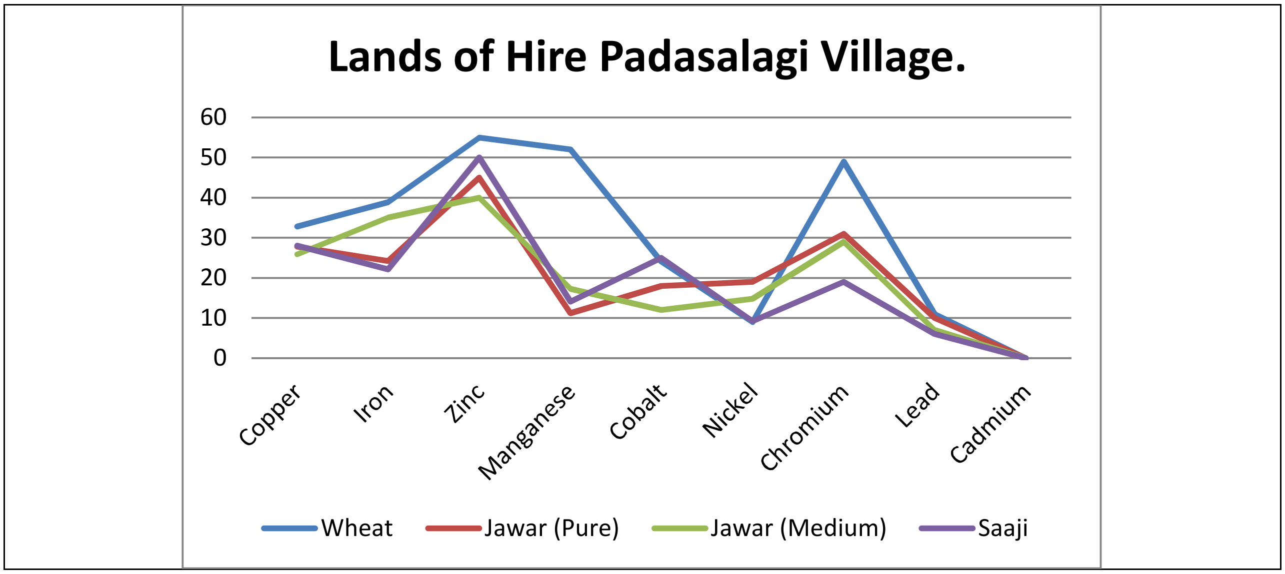

Fig.-3. Heavy Metals (ppm dry weight) in Cereals samples of Lands of Hire Padasalagi Village.

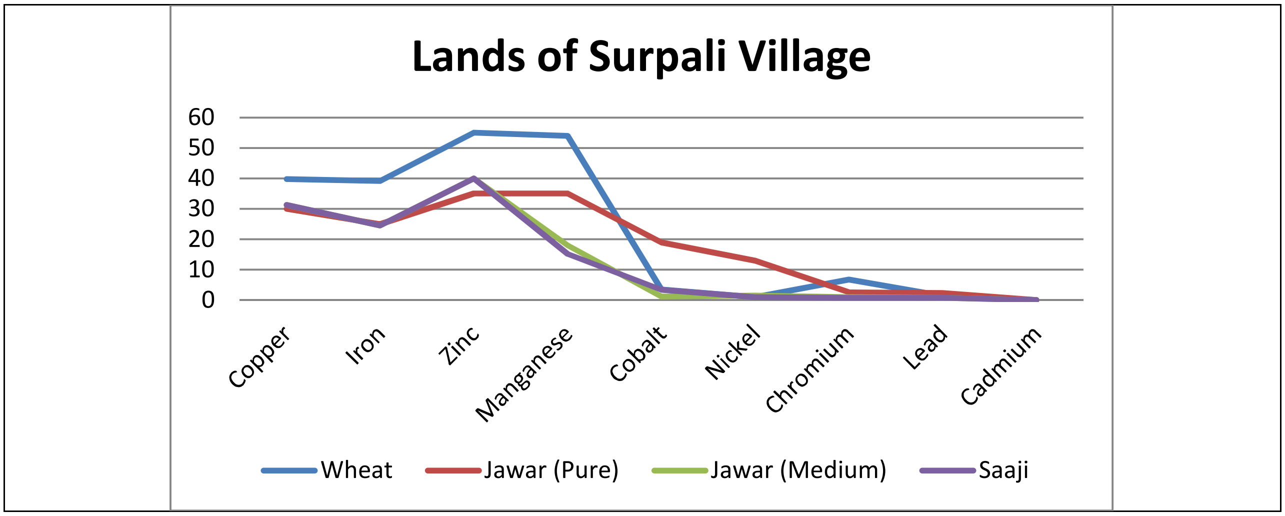

Fig.-4. Heavy Metals (ppm dry weight) in Cereals samples of Lands of Surpali Village.

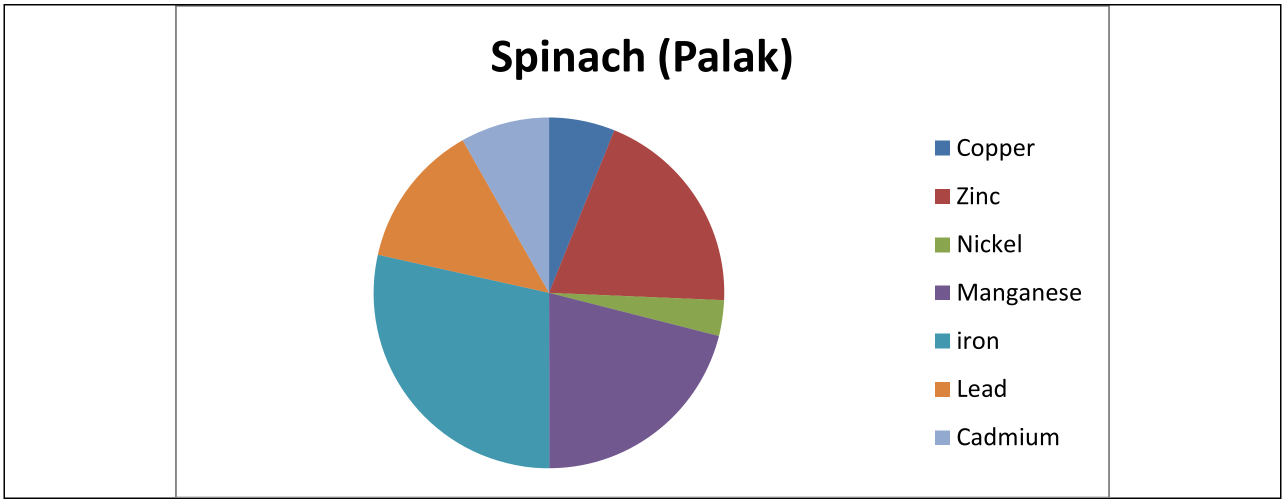

Fig.-5. Heavy Metals in Spinach (Palak) Green Vegetable (ppm value).

CONCLUSION

Analysis of heavy metal concentrations in cereals grown in soils of four selected villages irrigated with River Krishna water. The cultivation lands of Hipparagi is located nearer to the dumping spot (0.5 km) of municipal wastes / sewage wastes from Rabakavi and Banahatti Urbanized and Industrial towns to the stream of the river. In addition to this forming community were using fertilizers, pesticides for growing these cereals. Hence, the soil will be affected by the accumulation of these heavy metals. Most of the metals found in Wheat and Jawar grains were higher than the International standards. The villages like Surapali (4kms), Savalagi (8 kms) and Hire Padasalagi (11 kms) away from the municipal waste dumping spot. But, the heavy metal concentrations in the food grains (cereals) of the cultivation lands of these regions were found in higher ranges were due to agricultural practices, uses of fertilizers and pesticides. Zn, Fe, Cu in food grains in the current study of Hipparagi cultivated lands were found above the safe limit. Whereas Mn, Co, Ni, Cr, Pb and Cd were under the safe limits. The farming community of Hipparagi village and authorities of the municipal council of Rabakavi and Banahatti were informed and recommended that municipal waste water treatment must be carried out prior to dumping directly or indirectly into the stream of the river to avoid soil and food grains toxicity by heavy metals. The results reported here confirm that the vegetables collected from chosen production and marketplaces in the Jamkhandi city contained heavy metal contents within the safe limits prescribed by the WHO. But Lead, Cadmium and Iron exceeded the tolerance level. The concentration of Iron in Palak 1220.0 ppm, the concentration of Cd in Palak 31.6 ppm and the concentration of Lead in Sabasagi 58.1 ppm were highest and exceed the tolerance limit. The heavy metal concentration in available vegetables leads toxic effect to body system and causing health hazards.

Conflict of interest

It is quite necessary to educate the farming community providing information's, suggestions about the soil properties, recommendations made for proper uses of fertilizers and pesticides. The municipal authorities informed to go for proper treatment of municipal sewage water before dumping into the water stream. Formers were encouraged to reduce soil contamination by controlling the uses of fertilizers, pesticides.

ACKNOWLEDGEMENT

Authors express their sincere thanks to Dr. C.N.R. Rao, FRS National Research Professor, Chairman Vision Group on Science and Technology, Bangalore. The authors are also thankful to Dr. B.G.Mulinami former Vice-Chancellor and chief Administrative Officer, BLDE'S Association Vijaypur, authors are very grateful to Prof: S.H.Lagali Administrative Officer BLDE'S Association Vijaypur and Principal Dr. S. C. Hiremath for providing necessary facilities required to carry out this research work.

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[RJC-1575/2017]

RJC

RASĀYAN *J. Chem.*
Vol. 10 | No. 1 |165-175 | January - March | 2017
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

FLUORIDE TOXICITY ON HUMAN HEALTH FROM WATER RESOURCES AVAILABLE AT GRANITE MINE IN BAGALKOT DISTRICT, KARNATAKA, INDIA.

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ABSTRACT

Physico-Chemical analysis of ground water samples was carried out from 30 locations of Bagalkot district such as Hungund, Badami, Ron, Kustagi and Bagalkot taluks. The analysis of different parameters such as pH, EC, TDS, Cl, SO_4, NO_3 and Fluoride were carried out as per the standard methods. All the parameters studied were within the permissible limit except Fluoride content in few locations. The analyzed results indicate the Fluoride concentration in some sampling spots namely Herur, Kesarabhavi, Benekanadoni, Balakundi, and Husur of Hunagund Taluk. Maradi village, Budanagad locations of Badami Taluk. Hanumasagar, Hanumanal villages of Kustagi Taluk. Tulasigeri, Simikeri (Govt. Primary School Campus) of Bagalkot Taluk, were found above standards (WHO- 1.0 ppm to 1.5 ppm) probably due to seasonal variations and salt water contamination. Fluoride ion in water sources is known for both beneficial and detrimental effects on live stock. The higher concentration of Fluoride in ground water causes a disease called "Fluorosis". It is a slow, progressive, crippling malady, which affects every organ, tissue and cells in the body system and results in health complaints having overlapping manifestations with several other diseases like chronic dental and skeletal Fluorosis.

Keywords: fluoride toxicity, human health, granite mining, fluorosis effect on body organ, genetic material.

INTRODUCTION

Fluoride occurs in combined state, it is present naturally in almost all foods and beverages including water, but levels of which can vary widely. Fluoride in drinking water to adjust concentrations in between 0.8 ppm to 1.0 ppm for the beneficial effect of teeth decay prevention. The Fluoride accumulation of ground water varies according to the source of water, area with semi-arid, climate, crystalline rock and alkaline soils of the area. The types of rocks composition of the host rock that water flows through and amount of rain fall are mainly affected[1]. Fluoride is a geochemical contaminant and natural sources account for most of the Fluoride in surface and ground water[2]. Its concentration is dependent on solubility of Fluoride containing rocks.

Fluoride ion in drinking water is known for both beneficial and detrimental effects on health. World Health Organization and Indian council of Medical Research described the drinking water quality guidelines values for Fluoride is 1.5 ppm (Guidelines for drinking water quality International Standards for drinking water[3,4]. Low content ratio of Fluoride provides protection against dental caries, especially in children. In India around 60 million people including children were severely affected by Fluorosis because of high consumption of Fluoride content[5]. Longer exposure to Fluoride leads to certain types of bone diseases, mottling of teeth-enamel, nervous and skeletal disorder[6]. It also adversely affects the foetal cerebral function and neurotransmitters[7].

The number of people getting affected, meanwhile villages, blocks, districts and states endemic for Fluorosis have been steadily increasing ever since the disease was discovered in India during 1930s. The reason for the increase in the disease incidence and the sizeable number of locations being identified as endemic zones for Fluorosis is due to overgrowth of population, necessitating more and more water,

Rasayan J. Chem., 10(1), 165-175 (2017)
http://dx.doi.org/10.7324/RJC.2017.1011596

resorting to the use of hand pump water, unawareness regarding the importance of checking water quality especially for Fluoride content and due to water shortage. The agencies responsible for water supply (Municipal authorities) resort to pumping water from open wells bore wells to overhead tanks or direct supply to residents, and invariably such water sources are not tested for Fluoride[8].

Keeping in view of the above, the present investigation under taken to assess fluoride concentrations in water resources available around granite mining and various adverse effects on human health by estimating fluoride level in drinking water, identification of exact geographical locations which are having high concentration of fluoride in water, toxicity of fluoride due to the consumption of drinking water in the area of Bagalkot district of Karnataka state in India, especially in Hunagund, Ilakal, Badami and Bagalkot Taluk.

The main objectives of this research work was to investigate the various aspects of fluoride and its importance in human life, as well as fluorosis effect on young and old men and women alike. This investigation may help in bringing awareness about fluorosis diseases to the public residing in that affected area.

EXPERIMENTAL

Material and Methods

Water samples were collected from 30 locations from various villages in and around Bagalkot district. All the samples were stored at 25°C and analyzed by using a fluoride selective electrode (Thermo Scientific Arian, Combination Fluoride Electrode No. 9609 BNWP) as per the prescribed standard methods[9,10]. All the Physico-chemical parameters were measured in accordance with standard methods[11,12]. While collection of water samples, the temperature was recorded by 110th thermometer. All the Chemicals and reagents such as sodium fluoride, zyrconyl chloride, 3-alizerin sulphuric acid, ammonium acetate and other compounds used were of analytical grade. Double distilled water was used for preparing the required reagents and solutions.

Nitrate present in the water resources was measured by ion selective electrode method using digital ion-pH meter (Elico equipments pvt. Ltd., India) by taking known volume (25 ml) of water sample in 100 ml beaker and equal volume of buffer solution for total ionic strength adjustment was added and stirred for 1 minute. The electrode was immersed, recorded the readings when stable. pH, EC, TDS and other chemical parameters of water samples were also measured by electrode method. The chloride, alkalinity, total hardness, calcium, magnesium and sulphur in the form of sulphate were determined by titrimetric methods and turbidity methods[13].

All the parameter values were recorded in Tables-1 to 5, in different three seasons–during 2014–2015. These values were compared with the drinking water standards (table 6) of Bureau of Indian standards and World Health Organization for evaluation of Physico-chemical parameters, Nitrate ions and fluoride concentration in the water samples of the different locations were measured.

RESULTS AND DISCUSSION

It was observed that the water table depth found approximately in between 8 – 10 meters (in the selected locations based on the enquiry from the local people). All the 30 water samples being using for domestic purposes by the public were analyzed their quality parameters such as pH, EC, TDS, Cl, SO_4, nitrate and fluoride concentrations of the selected villages such as Belakundi of Hunagund Taluk, where the drinking water is supplying by the municipal board or by punchayat committee, through the water storage tanks. In addition to this the public of this area is also depended upon bore wells. But, in all locations, the water resources contaminated with the maximum fluoride concentration was noticed throughout the monitoring periods.

Temperature

The temperature of water is an important parameter because it effects bio-chemical reactions in aquatic organisms; rise in temperature reduces the solubility and amplifies the tests and odors. Hence, during summer days, DO values of water slightly decreases, the temperature of water and DO values are quite related. If the temperature of water reaches to 28°C to 29°C, the CO_2 gas begins to dissolve in water.

Hence, water turns to acidic and forms carbonic acid, as a result the pH of water changes. The alteration in pH of water is accompanied by change in other physicochemical aspects of the medium.
The study area of Hunagund and Ilakal is covered by granite. The area is semi-arid with subtropics climate conditions. The temperature varies in these locations 27.5°C to 29.8°C. The temperature of water samples were collected from the residential colonies situated in Bagalkot, Badami, Kustagi, Koppal and Ron in all three seasons were ranges in between 27°C to 29.0°C.

pH (Power of Hydrogen)

The pH is an important index of hydrogen ion activity and is resulting value of acid-base interaction of number of mineral and organic components in water. The pH is an important ecological factor used universally to express the intensity of acid and alkaline condition of the water samples. Most of the water samples in the present investigation were slightly alkaline in nature (pH 7.2 to 7.8) due to the presence of carbonates [CO_3] and bicarbonates [HCO_3]. Thus the pH values determine the equilibrium between free CO_2, CO_3 and HCO_3.
In the study locations like Cholachagudda village of Badami, Hanumanal and Hanumsagar villages of Kustagi, Kalliganur of Ron, the pH values of water samples ranges in between 6.8 to 7.1. Whereas the water samples collected from Belakundi, Herur and Benakanadoni of Hunagund, the pH values were found to be 8.1, 7.8 and 7.8 respectively. Hence, the water is alkaline in nature due to the presence of CO_3 and HCO_3. The pH values more than 7.0 in water samples reflect contamination of bases like sodium hydroxide and calcium hydroxide[14,15]. Nevertheless, no acidic water found around the granite mining.

Electrical Conductivity (EC)

It is an important parameter for determining the water quality for drinking and agricultural purposes. Many dissolved substances may produce an esthetically displeasing color, taste, odor and salinity conditions in water samples. It signifies the amount of total dissolved solids. The higher EC values in water samples indicate the presence of high amount of total inorganic substances in ionized state. EC value is always correlated with TDS found in water and EC is an indicator of degree of mineralization of water. In the present investigation the EC values ranged in between 0.746 m mhos/cm to 2.961 m mhos/cm in Hunagund locations of Bagalkot district, 1.460 m mhos/cm to 1.882 m mhos/cm in Kustagi Taluk of Koppal district, 0.486 m mhos/cm to 1.240 m mhos/cm found in the locations of Ron Taluk of Gadag district and EC values found in between 1.419 m mhos/cm to 1.747 m mhos/cm in Badami Taluk of Bagalkot district. Except Ron locations the EC values of all locations of water samples found slightly higher than the permissible limit (1.4 m mhos/cm) indicates the presence of maximum total dissolved solids in water samples of Hunagund, Kustagi and Badami taluks. Whereas the EC values of Ron taluk found within the legal limit prescribed by the international standards.

Total Dissolved Solids (TDS)

Total dissolved solids are one of the desirable parameters of water for drinking purpose. The TDS values of water samples were measured by using Elico TDS meter. TDS indicates the salinity behavior of ground water. Water containing more than 500 ppm of TDS is not considered desirable for drinking water supplies, but in unavoidable cases 1500 ppm is also allowed. In the present investigation the TDS values of Hunagund locations ranged in between 354 ppm to 1524 ppm the minimum TDS values found in the ground water of Hosur village, where as the maximum TDS values found in Herur village of the same Taluk. The TDS values 1127 ppm, 1071 ppm, 1081 ppm and 1217 ppm found in the bore well water samples of Chinnapur, Kesarabhavi, Mahanthpur and Tumba villages of Hunagund Taluk respectively, the water will give threat on the health of human and other beings. in case of Ron Taluk (Kuntoji, Gajendragad and Kalliganur villages) the TDS values of ground water samples found below the prescribed limits recommended by the WHO and ISI standards. TDS values in case Kustagi and Badami locations found slightly more than 500 ppm. People of this area are asked to use the water for drinking purposes after RO purifications.

Chloride (Cl)

Chloride serves as an indicator of pollution by sewage and industrial effluents. Chloride occurs in all ground waters, but in widely varying concentrations. Excessive chloride in potable water is not particularly harmful; however, chloride in excess (more than 250 ppm) imparts a salty taste to water. People accustomed to higher chloride in water are subjected to laxative effects. In the present investigation the chloride values ranged from 28.5 ppm to 37.8 ppm in the case of Kustagi Taluk of Koppal district. 26.6 ppm to 35.6 ppm found in Ron Taluk of Gadag district, and 27.6 ppm to 36.9 ppm from the water resources available in Badami Taluk of Bagalkot district. The maximum chloride concentration found in between 31.8 ppm to 54.5 ppm this is because of granite mines available around Hunagund Taluk of Bagalkot district.

Sulphate (SO_4)

Sulphate in the water samples is depending upon the nature of the soils. Each and every water resources consist with sulphate in varying ranges. It is known that the sulphate concentration in water samples around 1000 ppm has Laxative effect and causes gastrointestinal irritation. Excess sodium sulphate in water causes Cathartic action. The high concentration of Na and $MgSO_4$ is associated with respiratory illness. In the present investigation sulphate concentration in Hunagund locations found in between 28.6 ppm 63.5 ppm where as in Badami locations the sulphate concentration ranged in between 25.2 ppm to 56.3 ppm. The higher concentration of sulphate in Hunagund area due to granite rocks, iron and manganese ores. The sulphate concentration in the study area of Kustagi, Ron and Badami found less than the prescribed legal limits (WHO: 150 ppm to 250 ppm).

Nitrate (NO_3)

The water samples having Nitrate concentration below 22.5 ppm is said to be safe for agriculture uses, but higher than 22.5 ppm showed increasing problems on food products and vegetations. Thus, water from various locations whose Nitrate concentrations more than 22.5 ppm will be appeared to have gone in the increasing problem zone for agricultural purposes with regard to Nitrate concentrations. This is possibly due to unrestricted use of nitrogenous fertilizers in agricultural practices in the areas.

The analysis report reveals the Nitrate concentration is water samples collected from the locations of Hunagund of Bagalkot district found in between 14 ppm to 21.3 ppm. Where as in the locations of Badami and Ron range in between 11 ppm to 20.3 ppm and 12.3 ppm to 19.8 ppm respectively. Kustagi Taluk of Koppal district found Nitrate ion concentration 102 ppm to 18.9 ppm, all the vales were found within the prescribed legal limits.

Fluoride (F)

The major sources of Fluoride in ground water are fluoride bearing rocks such as fluorspar, Cryolite, Fluorspatite, granite rocks and hydroxyl apatite. Fluoride has widely been in the focus of public and scientific interest because of their important physiological role in the health of a man[16]. It is high time that an affordable solution should be found to minimize the fluoride contamination for maintaining the good health of the large population of the Hunagund, Ilakal, Bagalkot region of study area there is urgent need to carry out studies on hydro-chemical and hydro-geological aspect of occurrence of fluoride which can be useful to mitigate Fluorosis in the study area. Defluoridation tanks should also be installed in the villages which having high exposure of fluoride concentration in ground water resources where using for drinking purposes.

In the present investigation of water samples of Hunagund, Badami, Ilakal of Bagalkot district, Kustagi and Ron taluks in and around Bagalkot district out of 30 water samples 8 samples contained more Fluoride concentrations (above 2.4 ppm), the 7 water samples contained Fluoride concentration within the range of 1.5 ppm, and 4 water samples of study area consists with Fluoride concentration less than prescribed standard limit. The Fluoride concentration in the water samples of the villages such as Herur, Kesarabhavi, Benakanadoni Hosur and Balakundi of Hunagund taluk of Bagalkot district found in between 1.523 ppm to 2.433 ppm (Figures-1 and 3). Fluoride concentration in the ground water resources of Hanumasagar, Hanamanal villages of Kustagi Taluk found in between 1.524 ppm to 1.451 ppm (Figure-4). The least Fluoride concentration fond in the ground water resources of Jalihal, Belur and Cholachagudda villages of Badami Taluk in the Bagalkot district (Figure-2).

Picture-1: Dental Fluorosis caused by the uses of fluorinated bore water resources from Benakanadoni, Balakundi villages of Hunagund and Budangud village of Badami taluk.

Picture-2: Skeletal Fluorosis affected every organ of the body system (tissue, mental and nerves system) which results in health complaints (Locations: Hosur, Yerigonal & Kesarabhavi villages in and around Hunagund region).

Picture-3: Maximum Fluoride concentrations found in water resources of Hunagund, Ilakal and Badami taluks (Bagalkot District)

Higher concentration of Fluoride which is characterized by molting of teeth enamel, nervous and skeletal disorder (Picture-1 and 2). Ground water with high Fluoride content are generally Bicarbonates, sodium mixed water, particularly poor in Calcium content. Rocks which are rich in Fluoride mineral contributed enriched Fluoride contents of ground water. In the area of Bagalkot district the high levels of Fluoride are due to geogenic sources.

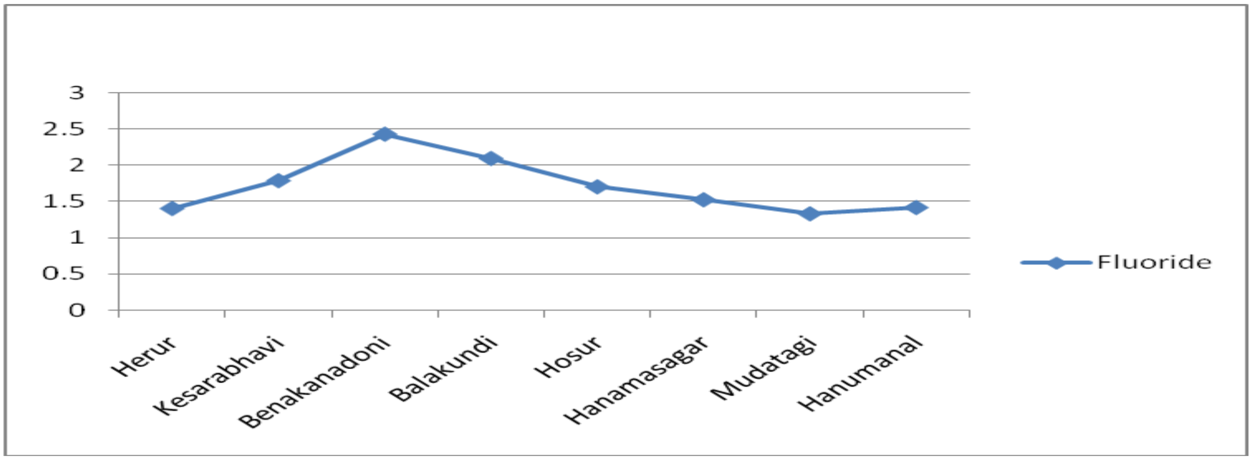

Fig.-1: Maximum fluoride content in Benakanadoni and Balakundi villages of Hunagund.

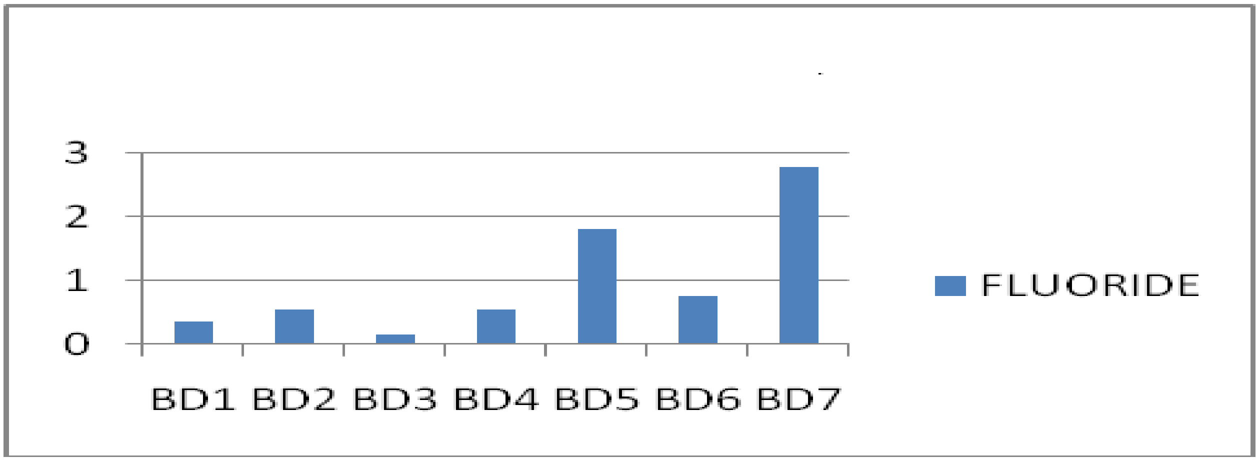

Fig.-2: Maximum fluoride content in Budangud village of Badami taluk. (Locations BD1 to BD7)

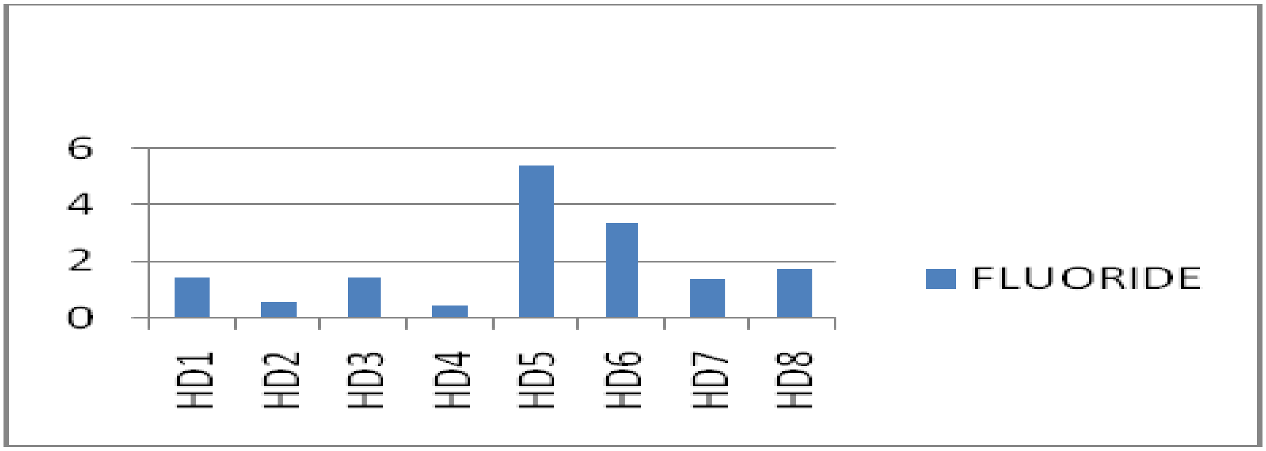

Fig.-3: Maximum fluoride content found in Yerigonal village in Hunagund region. (Locations HD1 to HD8)

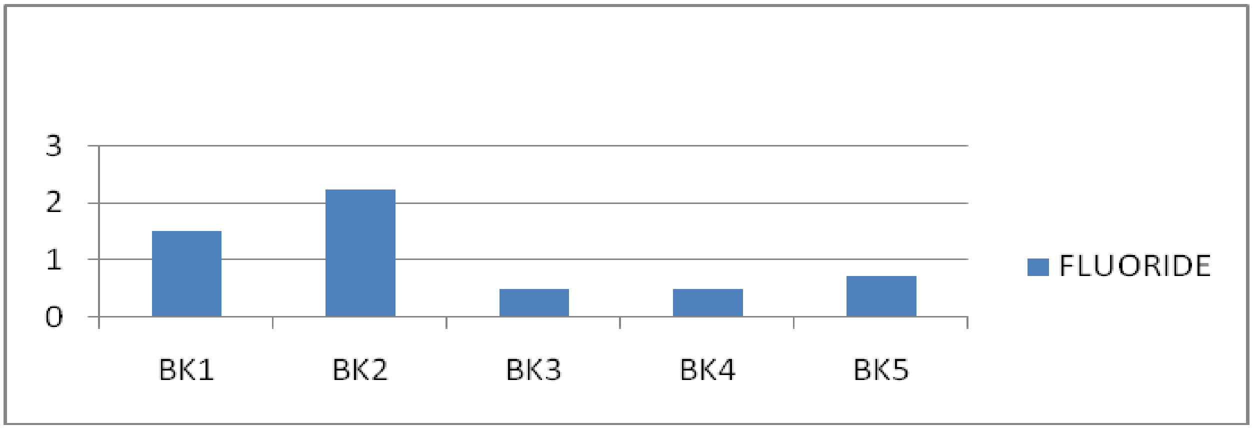

Fig.-4: Maximum Fluoride content found in ground water in Semikeri Village of Bagalkot District. (Locations BK1 to BK5).

Regular intake of Fluoride enriched waters seems to be the main cause for Fluorosis in the study area (Picture-3). These will be helpful to prepare Fluorosis plan for the affected population of the study area. It should be better to Monitoring systems is to be established to periodically evaluate the prevalence of fluorosis and dental carries in the affected areas. Documents of water fluoride concentration may be kept in municipalities/punchayat for the benefit of public health providers, health professionals and the public with regard to fluoride consuming from drinking water.

Defluoridation tanks should also be installed in the villages like Kesabhavi (pH 1.784), Benakadoni (pH 2.433), Balakundi (pH 2.096) Hosur (pH 1.703) of Hunagund Taluk and Jalihal H.K. village (pH 1.572), and Belur (pH 1.504) of Badami taluk. Around Bagalkot district some villages of Kustagi and Ron taluks are also affected by the kinds Fluorosis diseases, in these villages also having high exposure of Fluoride concentration in drinking water.

Table-1: Chemical parameters of water samples collected in and around Bagalkot district from the locations of Hunagund taluk during winter, summer and monsoon seasons of 2014-15

S.No.	Village & Taluk	Seasons	pH	EC m mhos/cm	TDS ppm	Cl ppm	SO_4 ppm	NO_3 ppm	Fluoride ppm
1	Herur of Hunagund	Winter	7.5	2.782	1296	30.2	27.8	17.3	1.503
		Summer	7.8	2.961	1396	31.8	28.6	18.6	1.523
		Monsoon	7.4	0.746	1125	30.1	26..8	17.8	1.421
2	Herur of Hunagund	Winter	7.2	2.864	1453	31.6	28.9	18.3	1.296
		Summer	7.2	2.961	1524	32.5	29.6	19.2	1.337
		Monsoon	7.1	1.956	1123	32.0	27.6	19.0	1.293
3	Chinnapur Hunagund	Winter	7.1	2.143	1056	42.3	30.5	19.6	1.301
		Summer	7.3	2.244	1127	44.1	31.2	20.1	1.367
		Monsoon	7.2	1.859	1005	41.3	31.0	18.9	1.323
4	Keasarabhavi Hunagund	Winter	7.6	2.048	1015	42.1	36.9	19.8	1.695
		Summer	7.8	2.150	1071	43.2	38.9	21.3	1.784
		Monsoon	7.7	1.986	989	40.6	35.4	19.3	1.761
5	Mahantapur Hunagund	Winter	7.4	2.017	987	32.	40.2	20.1	1.202
		Summer	7.5	2.149	1081	33.8	41.3	21.0	1.227
		Monsoon	7.3	1.968	995	31.6	40.9	19.4	1.201
	Tumba of Hunagund	Winter	7.2	2.147	1189	43.2	50.1	18.9	1.263
		Summer	7.3	2.396	1217	45.3	51.3	21.2	1.341
		Monsoon	7.1	2.004	1025	44.3	50.6	19.3	1.306
6	Benakanadoni Hunagund	Winter	7.8	0.811	325	52.9	61.2	19.5	0.896
		Summer	8.1	0.812	394	54.5	63.5	21.3	0.923

		Monsoon	7.6	0.789	301	52.6	62.6	20.3	0.854
7	Benakanadoni Hunagund	Winter	7.1	1.986	897	50.1	59.9	18.6	2.436
		Summer	7.8	2.028	996	53.2	62.5	19.2	2.443
		Monsoon	7.5	1.895	852	51.2	61.5	17.8	2.430
8	Balakundi Hunagund	Winter	7.9	0.857	412	50.1	27.9	16.7	1.986
		Summer	8.1	0.874	418	52.6	29.1	18.8	2.096
		Monsoon	8.0	0.789	396	51.6	28.9	15.8	1.963
9	Husur of Hunagund	Winter	7.5	0.698	325	43.2	29.5	16.5	1.639
		Summer	7.6	0.746	354	45.6	30.1	19.2	1.703
		Monsoon	7.4	0.668	301	41.5	28.9	17.3	1.693

Table-2: Chemical parameters of water samples collected in and around Bagalkot district from the locations of Badami taluk during winter, summer and monsoon seasons of 2014-15.

S.No.	Village & Taluk	Seasons	pH	EC m mhos/cm	TDS ppm	Cl ppm	SO_4 ppm	NO_3 ppm	Fluoride ppm
1	Jalihal H.K. Badami	Winter	7.5	1.321	789	25.6	24.6	10.6	1.153
		Summer	7.6	1.419	873	27.6	25.2	11.1	1.172
		Monsoon	7.4	1.228	812	26.8	25.0	10.8	1.135
2	Belur of Badami	Winter	7.2	1.536	698	33.2	45.3	14.6	1.210
		Summer	7.3	1.652	717	34.2	46.8	15.9	1.304
		Monsoon	7.2	1.455	696	33.9	45.9	14.6	1.223
3	Cholachagudda Badami	Winter	6.8	1.698	658	35.6	49.6	18.9	1.001
		Summer	6.8	1.747	700	36.5	56.3	20.3	1.109
		Monsoon	6.7	1.692	698	36.1	48.7	19.2	1.086
4	Maradi Badami	Winter	6.8	1.680	898	43	50	24	2.010
		Summer	7.6	1.461	925	67	32	26	2.800
		Monsoon	7.4	1.563	924	59	45	31	2.014
5	Budangad Badami	Winter	7.3	1.620	900	98	68	15	2.29
		Summer	7.5	1.610	900	95	54	18	2.80
		Monsoon	7.4	1.598	895	92	42	16	2.65
	Budangad Badami	Winter	7.5	1.660	912	72	48	11	3.34
		Summer	7.1	1.581	898	89	71	12	3.68
		Monsoon		1.485	852	78	56	12	3.58
6	Budangad Badami	Winter	7.2	1.640	918	88	38	27	3.55
		Summer	7.4	1.722	791	62	52	26	3.21
		Monsoon	7.1	1.652	786	75	48	23	3.25
7	Agasanakoppa Badami	Winter	7.1	1.510	778	28	25	21	0.34
		Summer	7.2	1.520	820	38	33	23	0.48
		Monsoon	7.3	1.598	789	35	35	22	0.52
8	Kerur of Badami	Winter	7.1	1.98	842	101	78	27	0.72
		Summer	7.0	1.95	821	82	62	23	0.53
		Monsoon	7.2	1.85	824	95	80	25	0.65
9	Guledagudda Badami	Winter	6.5	1.720	790	52	48	25	0.75
		Summer	6.9	1.642	798	110	40	22	0.82
		Monsoon	6.8	1.689	769	85	51	20	0.85

Table-3: Chemical parameters of water samples collected in and around Bagalkot district from the locations of Ron taluk during winter, summer and monsoon seasons of 2014-15.

S.No.	Village & Taluk	Seasons	pH	EC m mhos/cm	TDS ppm	Cl ppm	SO_4 ppm	NO_3 ppm	Fluoride ppm
1	Kuntoji of Ron	Winter	7.3	0.412	212	26.3	44.5	11.2	1.336
		Summer	7.4	0.486	228	26.6	45.6	12.0	1.377

		Monsoon	7.2	0.458	213	25.6	43.2	11.6	1.320
2	Gajendragad Ron	Winter	7.3	1.012	265	30.2	65.2	12.6	1.303
		Summer	7.4	1.120	273	32.5	66.2	14.3	1.306
		Monsoon	7.3	1.009	263	31.2	64.3	13.2	1.300
3	Kalliganur Ron	Winter	6.9	1.158	501	34.2	73.2	19.5	1.396
		Summer	7.0	1.240	598	35.6	72.6	20.1	1.422
		Monsoon	6.8	1.198	512	33.6	71.5	18.6	1.402

Table-4: Chemical parameters of water samples collected in and around Bagalkot district from the locations of Kustagi taluk during winter, summer and monsoon seasons of 2014-15.

S.No.	Village & Taluk	Seasons	pH	EC m mhos/cm	TDS ppm	Cl ppm	SO_4 ppm	NO_3 ppm	Fluoride ppm
1	Mudatagi Kustagi	Winter	7.4	1..352	659	27.8	59.6	19.9	1.320
		Summer	7.5	1.460	716	28.5	60.2	21.2	1.329
		Monsoon	7.3	1.356	649	27.6	56.8	18.6	1.301
2	Hanamasagar Kustagi	Winter	6.9	1.742	8.95	29.6	69.7	18.4	1.522
		Summer	6.8	1.882	9.38	30.2	71.3	20.5	1.524
		Monsoon	6.9	1.721	9.02	28.4	70.1	19.3	1.520
3	Hanamanal Kustagi	Winter	7.0	1.569	698	30.2	75.6	19.3	1.400
		Summer	7.1	1.622	797	34.5	82.3	22.0	1.416
		Monsoon	7.0	1.581	712	31.2	79.2	20.4	1.410
4	Hanamanal Kustagi	Winter	7.3	1.269	612	36.4	88.6	15.6	1.449
		Summer	7.4	1.385	677	37.8	91.5	19.5	1.451
		Monsoon	7.3	1.233	623	35.9	85.1	16.2	1.450

Table-5: Chemical parameters of water samples collected in and around Bagalkot district from the locations of Bagalkot taluk during winter, summer and monsoon seasons of 2014-15.

S. No.	Village & Taluk	Seasons	pH	EC m mhos/cm	TDS ppm	Cl ppm	SO_4 ppm	NO_3 ppm	Fluoride ppm
1	Tulasigeri Bagalkot	Winter	6.6	1.480	821	38	36	22	1.61
		Summer	6.7	1.510	790	21	28	13	1.50
		Monsoon	6.8	1.501	802	28	32	20	1.52
2	Semikeri Bagalkot	Winter	6.7	1.518	792	69	43	36	2.32
		Summer	6.6	1.683	786	52	36	21	2.23
		Monsoon	6.8	1.568	768	47	50	29	2.30
3	Muchandi Bagalkot	Winter	6.8	1.689	712	55	78	25	0.51
		Summer	6.8	1.360	634	48	62	20	0.47
		Monsoon	6.9	1.425	658	54	59	21	0.52
4	Sirur of Bagalkot	Winter	6.9	1.368	798	54	38	21	0.49
		Summer	6.7	1.570	723	36	42	18	0.48
		Monsoon	6.9	1.512	734	42	39	16	0.50
5	Mannikeri Bagalkot	Winter	6.7	1.720	698	78	71	24	0.78
		Summer	6.9	1.710	634	61	61	19	0.72
		Monsoon	6.8	1.698	686	72	70	22	0.80

Table-6: Prescribed legal limits and guidelines

Parameter	WHO	ISI	ICMR
pH	7.0 – 8.5	6.5-8.5	6.5-9.2
EC	1.4 ds/m	1400µs/cm	250
TDS	500	500	1500-3000
BOD	5.0	5.0	---
COD	10.0	10.0	---

DO	5.0	5.0	5.0
Cl’	250	250	1000
Calcium	75-100	45-75	200
Magnesium	30-150	30	50
Sodium	200	200	---
Potassium	1.4	1.4	---
Sulphate	150-250	150-200	400
TH	300	300	600
TA	120	200-600	200-600
Zinc	0.75	---	---
Copper	0.60	---	---
Iron	<1	0.3	---
Manganese	2.0	0.3	---
Nitrate	40-100	40-100	40-100
Fluoride	1.0-1.5	1.0-1.5	1.0-1.5
Color	5 HU	5 HU	5 HU
Odor	Unobjectionable	Unobjectionable	Unobjectionable
Turbidity	5 NTU	5 NTU	5 NTU

CONCLUSION

The present study attempted to identify the areas affected by fluoride contamination in ground water resources of Bagalkot, Badami, Hungund and Ilakal taluks and around Bagalkot. The taluks like Kustagi of Koppal and Ron of Gadag districts were also affected by the fluoride contaminated ground water resources. The study has focused more on both urban and rural areas of Bagalkot district in order to supplement the data base in this direction. The following conclusions, recommendations and suggestions are made based on the investigation:

1. De-fluoridation tanks should be installed in such area having high concentration of fluoride in ground water resources.
2. Fluoride concentrations can be diluted by inducing ground water recharge techniques, i.e., construction of percolation tanks, flooding of ground water by mixing surface water by promoting rain water harvesting.
3. The financial support by the Government is made to install water purification units in the fluorosis affected area.
4. The possibilities of bringing safe water from nearby villages can also be planned by the municipal and punchayat authorities.

ACKNOWLEDGEMENT

Authors express their sincere thanks to Dr. C.N.R. Rao, FRS National Research Professor, Chairman Vision Group on Science and Technology, Bangalore. Authors also take this opportunity to extend their sincere gratitude to the Chairman and Coordinator of Research and Development Centre Bharathiar University Coimbatore. The authors are very thankful to Dr. B.G.Mulinami former vice-Chancellor and chief Administrative Officer, Vijaypur, Prof: S.H.Lagali Administrative Officer BLDE’S Association Vijaypur and Principal Dr. S. C. Hiremath for providing necessary facilities required to carry out this research work.

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[RJC-1596/2017]

Original Article

Synthesis, Characterization, Antimicrobial, DNA cleavage, and Cytotoxicity Studies of Some Metal (II) Complexes of Tridentate Schiff Base Ligand: 2-hydroxy-3-((4-(4-phenylthiazol-2-yl) semicarbazide) methyl) Benzoic Acid

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ABSTRACT

Objective: The main aim of the present work was to synthesize a novel Schiff base ligand 2-hydroxy-3-((4-(4-phenylthiazol-2-yl) semicarbazide) methyl) benzoic acid is obtained by the condensation of N-(4-phenylthiazole-2-yl) hydrazine carboxamide with 3-Aldehydosalicylic acid and its Cu(II), Co(II), Ni(II), and Zn(II) complexes and study of their biological activity. **Methods:** The compounds are characterized by elemental analysis and various physicochemical techniques like IR, ^{1}H NMR, ESI-mass, and molar conductance data. All the compounds were screened for their antibacterial and antifungal activity by MIC method. Further, to study the *in vitro* cytotoxicity properties of all the compounds against Artemia salina and DNA cleavage activity by Agarose Gel Electrophoresis (AGE) method. **Results:** Spectral investigations suggested square pyramidal coordination geometrical arrangement for all the metal (II) complexes, having 1:1 stoichiometric ratio of the type [ML $(Cl)_2$]. The antimicrobial activity results revealed that the metal complexes were found to be more active than the free ligand. Furthermore, the DNA cleavage activity of the compounds on plasmid DNA *pBR322* molecule showed moderate activity. **Conclusion:** The newly synthesized ligand acts as OON donor tridentate chelate and coordinated through an oxygen of azomethine nitrogen, Phenolic OH and Carboxylic acid (COOH) of 3-Aldehydosalicylic acid to the Cu, Co, Ni and Zn metal ions and form square pyramidal geometrical arrangement. All the complexes are found to be non-electrolytic in nature. Further, all the newly prepared compounds showed moderate biological activity.

Key words: Transition metal complexes, Thaizole, Schiff base, Antimicrobial, DNA cleavage.

Submission Date: 10-04-2017;
Revision Date: 13-07-2017;
Accepted Date: 15-07-2017.

DOI: 10.5530/ijper.51.4.109

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INTRODUCTION

Medicinal chemistry has generated important interest in the design of metal complexes as potential diagnostic and therapeutic agents. Thiazoles are one of the most intensively investigated classes of aromatic five-membered heterocyclic and containing three carbons, one sulphur, and one nitrogen atom. Thiazole and its derivatives are very useful compounds in different fields of chemistry including medicine and agriculture. Many thiazole derivates such as bleomycin, abafungin, ritonavir, and sulfathiazole are well known potential biologically active compounds.[1] Also, thiazoles are the starting material for several compounds including dyes, fungicides, sulphur drugs, biocides and chemical reaction accelerators which exhibit microbial activity that can be well characterized by a large number of drugs in the market containing this moiety.[2] Schiff base complexes of transition metals are particular attention to inorganic chemists because of their structural, chemical and spectral properties are more strongly dependent on the nature of the ligand structure.[3-6] The coordination chemistry of transition metal complexes derived from Schiff base ligands have been among the majority widely studied coordination compounds in current years.[7,8] Since they are becoming increasingly important as analytical, biochemical and antimicrobial reagents and Metal complexes of O, S, and N-chelating ligands have more attracted considerable attention because of their interesting Physico-chemical properties, strong biological activities.[9-12] The fact, copper, calcium, magnesium, zinc, iron, chromium, molybdenum, and vanadium are fundamental metallic elements and exhibit great biological activity when associated with certain metal-protein complexes, participating in oxygen transport the storage of ions or electronic transfer reactions,[13,14] has created enormous interest in the study of systems containing theses metals.[15] Thiazole ring finds applications such as liquid crystals, fluorescent dyes, polymers, insecticides and antioxidants.[16,17] Therefore it has been found interesting to study the metal complexes containing thiazole moiety. Some of Schiff bases and their transition metal complexes have also been used as drugs as fungicidal, bactericidal, anti-tubercular and antiviral agent.[18,19] In current years, metal-based drugs have gained much importance in the medicinal field. They are used as medicines for the treatment of cancer, diabetes, cardiovascular diseases and anti-inflammatory.[20-22] The medical application of the metal complexes compounds of thiazole to impart strength, elasticity, and impermeability of water.[23] Analogous of hetero-aromatic Schiff base derived from 3-aldehydosalicylic acid have been to possess biological activity. Azomethine group (=C=N-) which is formed by the condensation of primary amines with aromatic aldehydes. Such Schiff base ligands containing various donor atoms like O, N, and S showed broad biological activities and they are bond to the metal ions of Cu (II), Ni (II), Zn (II), Co (II).[24-26] Based on these findings and in continuation of our research work on coordination chemistry, we have synthesized the new Schiff base ligand 2-hydroxy-3-((4-(4-phenylthiazol-2-yl) semicarbazide) methyl) benzoic acid containing the carbonyl, azomethine, and hydroxyl groups as potent chelating sites. In order to study the ligation behavior of this ligand, we have prepared a series of its Cu(II), Co(II), Ni(II) and Zn(II) complexes and characterized them by various physicochemical techniques and studied their antimicrobial, DNA cleavage and *In vitro* Cytotoxicity.

Experimental

Analysis and physical measurement

Elemental analysis(C, H, and N) was performed on Vario EL CHNS analyzer. IR spectra of the synthesized Schiff base and its metal complexes were recorded in KBr pellets on a Parkin-Elmer FT-IR instrumental in the range 4000-250 Cm^{-1}. ^{1}HNMR spectra of ligand and its Zn (II) complex were recorded on the FT-NMR spectrometer model Bruker Avance II, 400 MHz using d_6 DMSO as solvent. ESI-MS were recorded on a mass spectrometer equipped with electrospary ionization (ESI) source having mass arranged of 4000 amu in quadruple and 20000 amu in Tof. Molar conductivity measurement were recorded on ELICO (CM-180) conductivity bridge in DMF (10^{-3}) solution using a dip-type conductivity cell fitted with a platinum electrode.

Material and methods

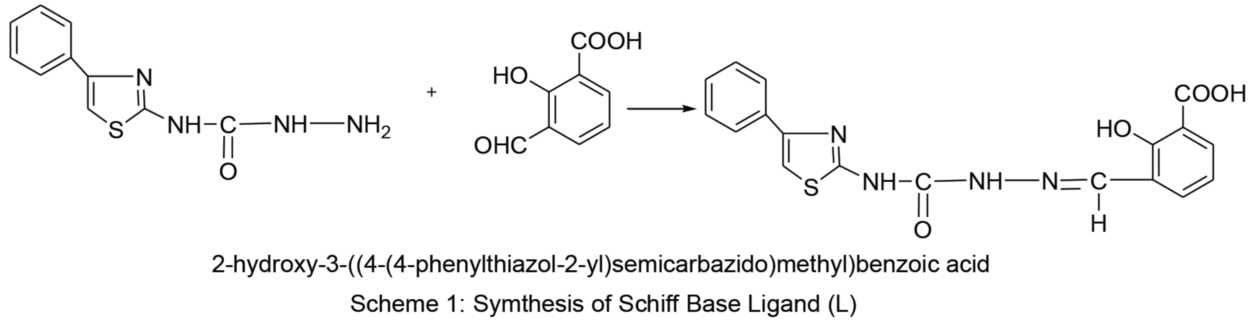
All reagents and chemicals required were AR grade, purchased commercially. All the solvents were purified by distillation and used. Thiourea, bromine, acetophenone, salicylic acid, hexamethylenetetramine, benzene, ammonium hydroxide, barium chloride, sodium hydroxide, hydrochloric acid and pyridine were purchased from S.D. Fine Chemicals, ethylchloroformate and hydrazine hydrate were purchased from Sigma Aldrich chemical company, India. Melting points of the newly synthesized compounds were determined by electro-thermal apparatus using open capillaries and are uncorrected. The metal and chloride contents of the metal complexes were determined as per standard procedures.[27] Purity of the compounds was checked by TLC and the spots were observed in iodine vapour. The precursor N-(4-phenylthiazol-2-yl) hydrazinecarboxamide was prepared by the literature method.[28]

Synthesis of Schiff base ligand (L)

An equimolar mixture of N-(4-phenylthiazol-2-yl) hydrazinecarboxamide (0.001 mol) and 3-Aldehydosalicylic acid (0.001 mol) in ethanol (30 ml) was refluxed with a catalytic amount of glacial acetic (1-2 drops) for about 5-6 hrs on a water bath, the yellow colored product which separated in hot was filtered off, washed with hot ethanol, dried and recrystallized from alcohol (Scheme 1). The reaction was monitored by TLC. Yield: 72% M.P: 267-280^{0}C.

Synthesis of metal (II) complexes

To the 2-hydroxy-3-((4-(4-phenylthaizole-2-yl) semicarbazido) methyl) benzoic acid (0.001 mol) in ethanol (25 ml) was added hot ethanolic solution (20ml) of respective metal chlorides (0.001 mol). The reaction



Scheme 1: Synthesis of Schiff base ligand (L).

mixture was then refluxed on water bath for about 4-5 hrs, pH of the reaction mixture adjusted Ca. 7 to 7.5 by adding alcoholic solution of sodium acetate (0.5 gm) and refluxing continued for about an one hr more. The reaction mixture was cooled to room temperature and poured into distilled water. The colored solids separated were collected by filtration, washed with sufficient quantity of distilled water, then with hot ethanol to remove any traces of unreacted starting materials and finally dried in a vacuum over anhydrous calcium chloride in desiccator.

Biological activities

Antimicrobial assays

The biological activities of the newly synthesized ligand and their Cu (II), Co (II), Ni (II) and Zn (II) complexes were screened for their antibacterial and antifungal activities by disc and well diffusion method respectively.[29]

The *in vitro* antibacterial activities of the compounds were tested against two Gram-negative [*Escherichia coli and Salmonella typhi*] and two Gram-positive [*Bacillus subtilis and Staphylococcus aureus*] bacteria. The *in vitro* antifungal activities were carried out against *Candida albicans, Cladosporium oxy-sporum and Aspergillus Niger fungi*. The stock solutions of the test chemicals (1 mg mL^{-1}) were prepared by dissolving 10 mg of the each test compound in 10 mL of freshly distilled DMSO. The different concentrations of the test compounds (100, 50, 25 and 12.5 μg mL^{-1}), were prepared by diluting the stock solution with the required amount of distilled DMSO. The lowest concentration that inhibited microbial growth was called as the MIC value. Further the dilutions for the metal chlorides were prepared by using distilled water and control experiments were carried out by using DMSO solvent alone.

Antibacterial screening

Muller–Hinton agar media was used for the antibacterial studies. The pure dehydrated Muller–Hilton agar (38 g) was dissolved in 1000 mL distilled water. The pure cultures of the bacterial strains *E. coli, S. aureus, B. subtilis and S. typhi* were sub cultured by inoculating them in the nutrient broth and they were incubated at 37^0C for about 18 h. The agar plates were prepared by using the above media. Each plate were inoculated with 18 h old bacterial culture (100 μL) using a micropipette and spread uniformly using bent glass rod. Wells were dug with the help of 6 mm sterile metallic cork borer. The drug *gentamycin* is used as standard. Different concentration of the test compounds and their respective metal chloride solutions were incorporated into the wells using micropipette and the plates were kept for incubation at 37^0C for 24 h. Soon after the completion of incubation period, the diameter of the inhibition zone generated by each test compound against bacterial growth were measured using antibiogram zone measuring scale.

Antifungal screening

Potato dextrose agar (PDA) media was used for the antifungal studies. The following ingredients were used to prepare the media i.e. potatoes (sliced washed unpeeled) 200 g, dextrose 20 g, agar 20 g in 1000 mL distilled water. The pure cultures *C. albicans, C. oxysporum and A. niger* were inoculated on PDA slants. These slants were incubated at 32^0C for 7 days. To these 7 days old slants of fungal strains, 10 mL of 0.1% tween-80 solution was added and the culture were scraped with sterile inoculating loop to get uniform spore suspension. The agar plates were prepared by using the above potato dextrose agar media. Each plate were inoculated with 7 days old spore suspension of each fungal culture (100 μL) using a micropipette and spreaded uniformly using bent glass rod. Wells were dug with the help of 6 mm sterile metallic cork borer. Each well was incorporated with the test compound solution of different concentrations and their respective metal chloride solution. The drug *Fluconazole* is used as standard. All the inoculated plates were incubated at 32 ^{0}C for about 48 h. Soon after the completion of incubation period the diameter of the inhibition zone generated by each test compound against fungal growth were measured using antibiogram zone measuring scale.

DNA cleavage experiment

The extent to which the newly synthesized ligands and their metal complexes could function as DNA cleavage agents was examined using supercoiled plasmid *DNA pBR 322* (Bangal re Genei, Bengaluru, Cat. No.105850) as a target molecule. The electrophoresis method was employed to study the efficiency of cleavage by the synthesized compounds. Each test compounds (100 μg) were added separately to the 225 mg *pBR 322 DNA* sample and these samples mixtures were incubated at 37 ^{0}C for 2 h. The electrophoresis of the test compounds was done according to the literature method.[30] Agarose (600 mg) was dissolved in hot tris-acetate-EDTA (TAE) buffer (60 mL) (4.84 g Tris base, pH – 8.0, 0.5 M EDTA L^{-1}) and heated to boil for few minutes. When the gel attains approximately 55 ^{0}C, it was then poured into the gas cassette fitted with comb. Slowly the gel was allowed to solidify by cooling to room temperature and then carefully the comb was removed. The solidified gel was placed in the electrophoresis chamber containing TAE buffer. The DNA sample (20 μL) initially treated with the test compounds were mixed with bromophenol blue dye in equimolar ratio along with standard DNA marker containing TAE buffer was loaded carefully into the wells and the constant 50 V of electricity was supplied for about 30 min. Later, the gel was removed, stained with Ethidium bromide solution (10 μgml^{-1}) for 15–20 min and then the bands were observed and photographed under UV-illuminator.

In vitro Cytotoxicity

Brine shrimp nauplii (Artemia salina) be used in the *in vitro* cytotoxicity analyze, according to the protocol of Meyer *et. al.*[31] with some modifications. This is a rapid, efficient, inexpensive test and has a good relationship with cytotoxic activity. *Brine shrimp (A. salina)* eggs was hatch in a shallow rectangular plastic dish (22 x 32 cm) packed with artificial seawater, which was prepared with a mixture of commercial salt and double distilled water. An unequal partition was made in the plastic dish with the help of a perforated apparatus. Approximately 50 mg of eggs are sprinkled into the large compartment, which has darkened while the small compartments were open to ordinary light. Two days after nauplii were collected by pipette by lighted side. Samples of the test compound were prepared by dissolving 20 mg of each compound in 2 ml of DMSO. From the stock separate vials and the volume of each vial made up to 10ml with artificial sea water to obtain the desired final concentrations. The negative control was prepared in the same manner, omitting the sample. After two days, when shrimp larvae were ready, 10 shrimp nauplii were then placed in each vial. After 24 hrs incubation, the vials were observed using a magnifying glass, and the number of survivors in each vial was counted. Tests were performed in triplicate and the resulting data were analyzed by a Finney computer program to determine the LD_{50} valves.[32] The results for test compounds were compared with positive control bleomycin.

Results and discussion

The newly synthesized metal complexes are colored solids, stable at room temperature and possess high melting point (>278^{0}C). The metal complexes are insoluble in water and common organic solvents but completely soluble in DMF and DMSO. The evidence for the formation of tridentates OON donor nature of the Schiff base ligand (L) was confirmed by using various spectral techniques. Elemental analysis and analytical data (Table 1) agree well with the proposed composition of Schiff base ligand and its metal complexes. These data of metal complexes suggest that the metal to ligand ratio of the complexes is 1:1 stoichiometry of the type $[M (L) (Cl)_2]$ for Cu (II), Co (II), Ni (II) and Zn (II) complexes. The measured molar conductance values of the metal complexes were too low to account for any dissociation of the complexes in DMF (18–36 ohm^{-1} cm^2 $mole^{-1}$), indicating their non-electrolytic behavior.[33]

IR spectral studies

Infrared spectra helps in getting on idea on how is the ligand coordinate to metal ion. The characteristics frequencies of the expected functional groups are depicted in Table 2. IR spectrum of the ligand showed a high intensity band at 1727 cm^{-1} due to carbonyl function (C=O) and two absorption bands at 3259 cm^{-1}, 3119 cm^{-1} due to amide NH and NH attached to thiazole moiety respectively. A high intensity band observed at 1628 cm^{-1} is attributed to the azomethine (C=N) vibration. IR spectrum of Schiff base ligand showed a broad band at 3176 cm^{-1} and 3480 cm^{-1} due to phenolic OH and COOH respectively Figure 1.

The IR spectra of the metal complexes exhibited ligand bands with the appropriate shifts due to complex formation. In the IR spectra of all the metal complexes it was observed that, the absence of band at 3176 cm^{-1} and 3480 cm^{-1} due to phenolic OH and COOH of ligand indicates the formation of coordination bond between the metal ions. IR spectrum of the metal complexes, medium intensity weak bands at 3240-3180 cm^{-1} and 3104-3080 cm^{-1} were due to amide NH and NH

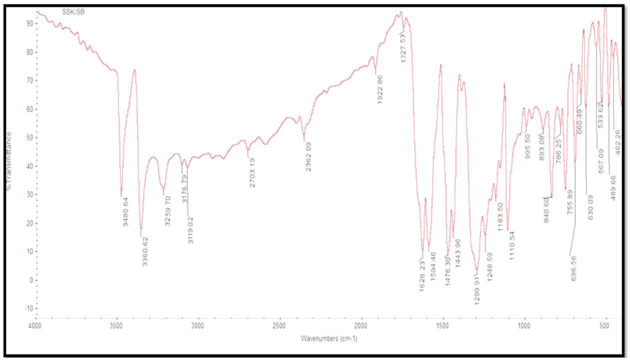


Figure 1: IR Spectrum of Schiff base ligand

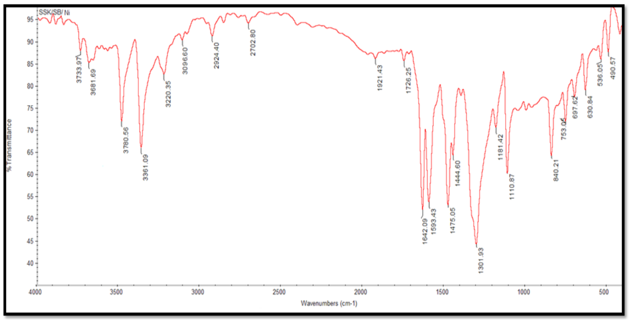


Figure 2: IR spectrum of Ni (II) complex

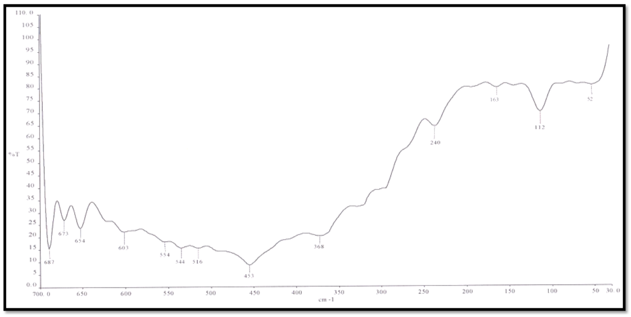


Figure 3: Far –IR spectrum of Cu (II) complex

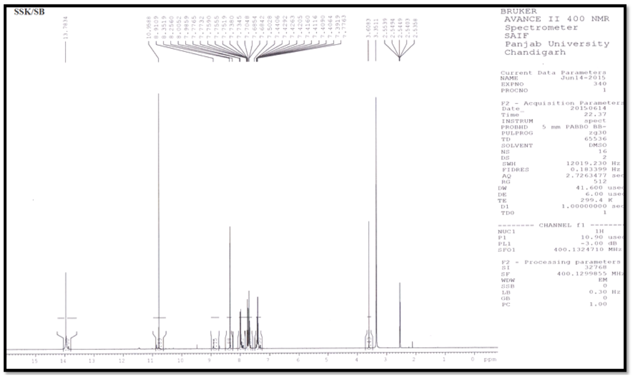


Figure 4: ^{1}NMR spectrum of Schiff base ligand

attached to thiazole moiety respectively, which appeared almost at about the same position as in the case of ligand, thus confirming their non-involvement in coordination. The IR spectrum all the complexes showed a shift of the azomethine (C=N) band towards lower frequency side about 68-26 cm^{-1} and appeared in the region 1594-1556 cm^{-1} when compared with the free ligand indicating the coordination of the azomethine nitrogen to the metal ion.[34] The shift amide carbonyl (C=O) to lower frequency side which appear in the region same position as in case of ligand, thus confirming non involvement in coordination Figure 2. The formation of metal complex was further confirmed by the appearance of new bands in the region 542-514, 489-448 and 327-312 cm^{-1} in all the complexes due to skeletal metal-oxygen, metal-nitrogen and metal-chlorides vibrations respectively Figure 3.

^{1}H NMR

The ^{1}H NMR spectra data of Schiff base ligand (L) and its Zn (II) complex were recorded in d6-DMSO and depicted in Table 3. The ^{1}H NMR spectrum of ligand displayed five distinct singlet at δ 13.59 ppm (s, 1H, Carboxylic acid), δ 12.2 ppm (s, 1H, Phenolic OH), δ 10.70 (s,1H, CONH), δ 8.93 (s, 1H, CONH), δ 8.38 (s,1H, CH=N) and 9 aromatic protons as multiplets in the region of δ 7.39-8.40 (m,9H,ArH) Figure 4. In the ^{1}H NMR spectrum of Zn (II) complex showed the disappearance of signal due to protons of carboxylic acid and phenolic OH confirms the involvement of bonding to metal ion via deprotonation. The ^{1}H NMR of Zn (II) complex displayed three distinct singlet at δ 9.23(s, 1H, CONH), δ 8.38 (s, 1H, CONH) and 8.20 (s, 1H, CH=N) and 9 aromatic protons as multiplets in the region 7.07-8.10 (m, 9H, ArH). When compared to the ^{1}H NMR spectrum of Schiff base ligand and its metal complex, it was found that the signals due to the amide NH, NH attached to thiazole, azomethine proton and aromatic protons have been shifted towards down field strength confirming the complexation of Zn (II) ion with ligand.[35] Figure 5.

ESI- mass spectral studies

The ESI mass spectra of the Schiff base ligand (L) and its Cu (II), and Co (II) complexes have been studied for their mass spectral studies. The ESI-mass spectra of the compounds exhibited molecular ion peaks equivalent to their molecular weight along other fragment peaks Figure 6. The ESI mass spectrum of the Schiff base ligand (L) showed a molecular ion peak recorded at m/z 382 which is equivalent to its molecular weight. Similarly, the ESI mass spectra of Cu (II) and Co (II) complexes

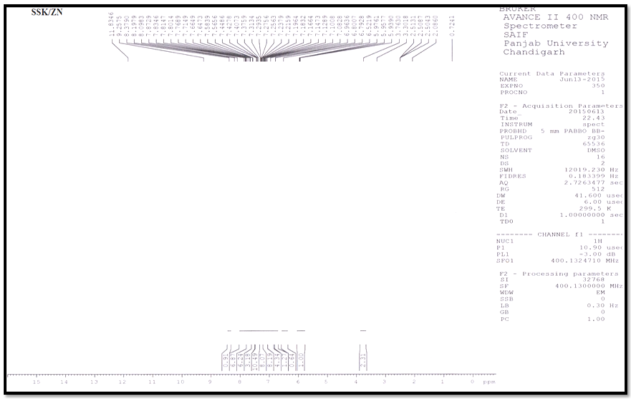


Figure 5: ^{1}NMR spectrum of Zn (II) complex

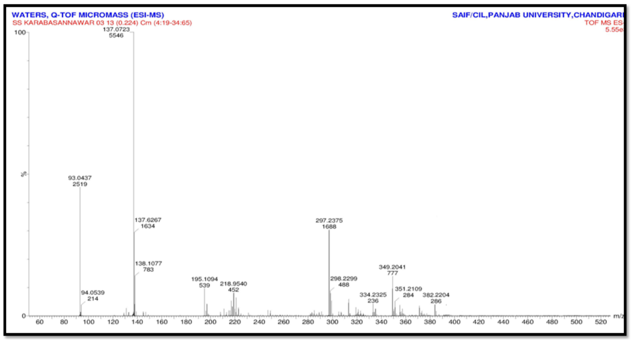


Figure 6: ESI Mass Spectrum of Schiff Base Ligand

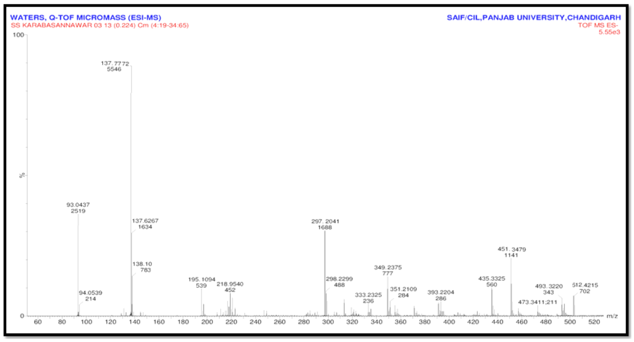


Figure 7: ESI Mass Spectrum of Cu (II) complex

showed a molecular ion peaks recorded to m/z 512 and 508 respectively which are equivalent to their molecular weights Figure 7.

Biological Activities

In vitro antimicrobial activity

The synthesized ligand and their metal complexes have been screened for their antimicrobial activity. The antimicrobial activities were carried out against *Escherichia coli, Salmonella typhi, Bacillus subtilis and Staphylococcus aureus* bacterial strains and anti fungal activity against *Candida albicans, Cladosporium oxy-sporum and Aspergillus niger* fungal strains. The antimicrobial activity results and minimum inhibitory concentration values of the compounds against respective strains are summarized in Table 4. the antimicrobial activity results of all the synthesized compounds exhibit antimicrobial properties and it is important to note that the metal complexes exhibited more inhibitory effect compared to their respective ligands and their metal chlorides. The enhanced antimicrobial activity of the complexes over the ligands and their metal chlorides can be explained on the basis of chelation theory.[36,37] It is known theory chelation enhances the ligand to act as more powerful potent bacterial agents, thus killing more of the bacteria than the ligand. The enhancement in the activity may be rationalized on the basis that ligands mainly possess azomethine (C=N) bond. It has been suggested that the ligands with hetro donor atoms (nitrogen and oxygen) inhibit enzyme activity, since the enzymes which require these groups for their activity appear to be especially more susceptible to deactivation by metal ion on coordination. It is observed that, in a complex, the positive charge of the metal ion is partially shared with the ligand and there may π-electron delocalization over the whole chelating system.[38] Thus the increase in the lipophilic character of the metal chelates and favors its permeation through the lipoid layer of the bacterial membranes and blocking of the metal binding sites in the enzymes of microorganisms. The factors namely solubility, conductivity and bond length between the metal ion and the ligand also increases the activity. The increase in the activity of metal complexes against the fungi is due to the formation of a hydrogen bond the azomethine nitrogen atom and active centers of the cell constituents, resulting in the interference with the normal cell process.

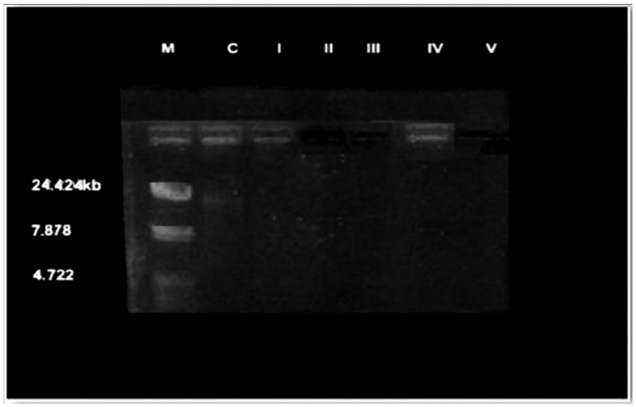


Figure 8: DNA cleavage of super coiled plasmid DNA pBR322. M, standard molecular weight marker; C, control. Ligand (Lane I) and its Cu (II), Co (II) and Ni (II) (Lane II, III and IV) were treated plasmid DNA pBR322 with respective compounds.

DNA cleavage activity

The ligand and its Cu(II), Co(II), Ni(II) and Zn(II) complexes were studied for their DNA cleavage activity by agarose gel electrophoresis method against supercoiled DNA pBR 322 (Bangal re Genei, Bengaluru, Cat.No.105850) as a target molecule and the gel picture showing cleavage is depticted in Figure 8. The characterization of DNA recognition by transition metal complex has been aided by the DNA cleavage chemistry associated with redox active or photo- activated metal complexe.[39] The electrophoresis analysis clearly revealed that the ligand and its metal complexes have acted on DNA because of a difference in molecular weight between the control and the treated DNA samples. The difference was observed in the bands of lanes of complexes compared with the control DNA (lane C) of *pBR322* due to the relaxation of circular DNA into linear form. This shows that the control DNA alone does not show any apparent cleavage, whereas the ligand and its metal complexes do show. In the present case, the ligand(Lane I) and its Cu (II), Co (II) and Ni (II) (Lane II, III and IV) complexes showed complete cleavage of supercoiled DNA whereas Zn (II) complex showed partial cleavage of supercoiled DNA. It can be concluded that all the compounds under present study inhibited the growth of pathogenic organisms by DNA cleavage as has been observed on the DNA cleavage of supercoiled plasmid DNA pBR322.

In vitro Cytotoxicity

The brine shrimp bioassay is an excellent tool to be used for monitoring the biological activity in order to predict the ability to kill cancer cells.[40] A summary of the cytotoxic assay results of the Schiff base ligand (L)

Table 1: Physical, Analytical and Molar conductance data of Schiff base ligand (L) and its metal complexes

Compounds	M.W.[a]	M.P (^{0}C) [b]			Elemental analysis found [%]					λ ($cm^2\Omega^{-1}mol^{-1}$)	Color
			M	C	H	N	O	S	Cl		
$C_{18}H_{14}N_4O_4S$	382.4	274-280	-----	56.54	3.69	14.65	16.74	8.39	-----	-----	Yellow
[Cu($C_{18}H_{12}N_4O_3S$) Cl_2]	498.8	286	12.74	43.34	2.42	11.23	9.62	6.43	14.21	24	Green
[Co($C_{18}H_{12}N_4O_3S$) Cl_2]	494.2	290	11.92	43.74	2.45	11.34	9.71	6.49	14.35	18	Brown
[Ni($C_{18}H_{12}N_4O_3S$) Cl_2]	494	285	11.34	43.77	2.45	11.34	9.72	6.49	14.35	36	Brown
[Zn($C_{18}H_{12}N_4O_3S$) Cl_2]	500.7	287	13.06	43.18	2.42	11.19	9.59	6.40	14.16	30	Pale Yellow

[a] molecular weight of the compounds

[b] melting point if the compounds at their decomposition

Table 2: IR spectral data of Schiff base ligand and its metal complexes

Compounds	Amide NH	Thiazole NH	C=O	C=N	OH	COOH	M-O	M-N	M-Cl
$C_{18}H_{14}N_4O_4S$	3259	3119	1727	1628	3176	3480	-----	-----	-----
[Cu($C_{18}H_{12}N_4O_3S$) Cl_2]	3229	3104	1726	1591	-----	------	542	495	368
[Co($C_{18}H_{12}N_4O_3S$) Cl_2]	3221	3096	1727	1594	-----	------	533	489	360
[Ni($C_{18}H_{12}N_4O_3S$) Cl_2]	3220	3096	1726	1593	-----	------	536	497	337
[Zn($C_{18}H_{12}N_4O_3S$) Cl_2]	3225	3063	1726	1556	-----	------	546	496	326

Table 3: ^{1}HNMR data of Schiff base ligand (L) and its Zn (II) metal complexes

Ligand / complex	^{1}H NMR data (ppm)
$C_{18}H_{14}N_4O_4S$	13.59 (s, 1H, Carboxylic acid) 12.2 (s, 1H, Phenolic OH) 10.70 (s,1H, NH attached to thiazole) 8.93 (s, 1H, CONH) 8.38 (s,1H, CH=N) 7.39-8.40 (m, 9H, ArH).
[Zn($C_{18}H_{12}N_4O_3S$) Cl_2]	9.23(s, 1H, NH attached to thiazole) 8.38 (s, 1H, CONH) 8.20 (s, 1H, CH=N) 7.07-8.10 (m, 9H, ArH)

Table 4: Minimum inhibitory concentration (MIC μg mL^{-1}) of Schiff base ligand and its metal complexes

Compounds	Bacteria				Fungi		
	S.aureus	B.Subtilis	E.coli	S.typhi	C.albicans	C.oxysporum	A.niger
$C_{18}H_{14}N_4O_4S$	50	75	75	50	75	75	50
$[Cu(C_{18}H_{12}N_4O_3S)\ Cl_2]$	50	25	50	25	50	25	50
$[Co(C_{18}H_{12}N_4O_3S)\ Cl_2]$	25	50	25	50	25	50	25
$[Ni(C_{18}H_{12}N_4O_3S)\ Cl_2]$	50	25	50	50	50	25	50
$[Zn(C_{18}H_{12}N_4O_3S)\ Cl_2]$	50	50	50	50	25	50	25
Gentamicin	12.50	12.50	12.50	12.50	--	--	--
Fluconazole	--	--	--	--	12.50	12.50	12.50

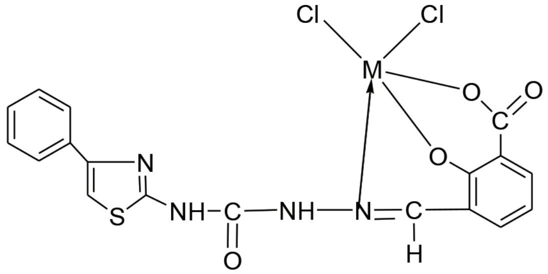
Table 5: Brine shrimp bioassay data of the Schiff base ligand (L) and its metal complexes

Compounds	LD50(M/mL)
$C_{18}H_{14}N_4O_4S$	2.276×10^{-4}
$[Cu(C_{18}H_{12}N_4O_3S)\ Cl_2]$	2.187×10^{-4}
$[Co(C_{18}H_{12}N_4O_3S)\ Cl_2]$	1.104×10^{-4}
$[Ni(C_{18}H_{12}N_4O_3S)\ Cl_2]$	2.321×10^{-4}
$[Zn(C_{18}H_{12}N_4O_3S)\ Cl_2]$	1.145×10^{-4}

and its metal complexes is presented in Table 5. The standard anticancer drug bleomycin showed the LD_{50} value $0.51X10^{-4}$. Among all the compounds tested Co (II) complex showed the highest cytotoxicity with LD_{50} value of $1.108X10^{-4}$ which is indicative of its potent cytotoxicity than other coordination complexes in this experiment showed followed by Zn (II) complex with LD_{50} value of $1.156X10^{-4}$. On the other hand, ligand (L), Cu (II) and Ni (II) complex were found to be inactive against A.salina.

CONCLUSION

The newly synthesized Schiff base ligand 2-hydroxy-3-((4-(4-phenylthiazol-2-yl) semicarbazide) methyl) benzoic acid behaves as tridentate OON donor and the complexes of square pyramidal coordination type $[ML\ (Cl)_2]$. The help of various physicochemical and spectroscopic methods such as IR, ^{1}H NMR, the square pyramidal coordination geometries of Cu (II), Co (II), Ni (II), and Zn (II) complexes have been proposed (**scheme 2**). The non-electrolyte nature of the complexes was confirmed on the basis of their molar conductance values. The newly synthesized metal complexes having good antimicrobial activity when compared to Schiff base ligand. The DNA cleavage activity of all the newly synthesized compounds showed the cleavage of plasmid DNA cleavage. In addition to that, cytotoxicity of Co (II) and Zn (II) complexes indicate potent cytotoxic agents that might become potent anticancer agent in clinical trials. Hence from all these extensive observations; it was concluded that the Schiff base ligand (L) and its metal complexes give the significant, adaptable and valuable information of coordination compounds and also they may be used as potent biological agents with reduced toxicity and higher efficiency.



M= Cu (II), Co (II), Ni (II), and Zn (II)

Scheme 2: Proposed structure of the complexes.

ACKNOWLEDGMENT

Authors are thankful to Principal, HOD Department of chemistry BLDE's science college Jamkhandi, Karnataka, India for providing necessary facilities for research. Authors are extended their thanks to professor, chairman of department chemistry and Coordinator of Research and development centre Bharathiar University Coimbatore. Authors are also thanks to SAIF Punjab University, Chandigarh, for providing FT-IR, ^{1}H NMR and ESI mass spectral data, and Biogenic Research and Training Centre in Biotechnology, Hubli, for Biological analysis.

CONFLICT OF INTEREST

No conflict of interest are declared.

ABBREVIATION USED

FT-IR: Fourier Trans- form Infrared; **^{1}H NMR:** Proton Nuclear Magnetic Resonance; **ESI mass:** Electrospray Ionization Mass Spectrometry; **DNA:** Deoxyribonucleic acid; **TLC:** Thin-layer chromatography; **DMSO:** Dimethyl sulfoxide; **TMS:** Tetramethylsilane; **DMF:** Dimethylformamide; **MTCC:** Microbial Type Culture Collection and Gene Bank; **PDA:** Potato dextrose agar; **EDTA:** Ethylene diamine tetraacetic acid; **MIC:** Minimum inhibitory concentration; **LD50:** Lethal Dose; **ETBr:** Ethidium bromide.

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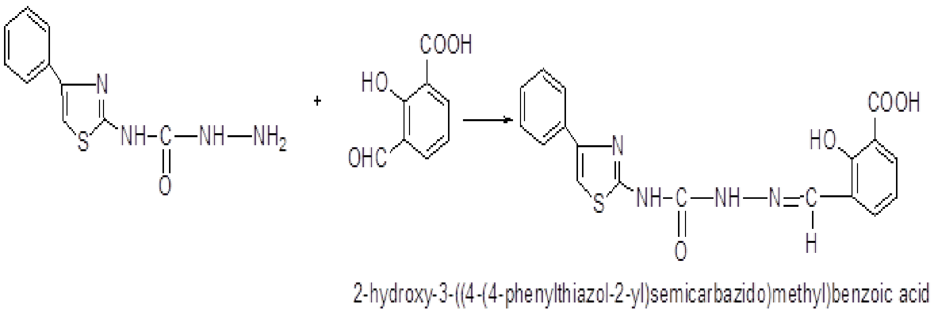
PICTORIAL ABSTRACT



SUMMARY

- The newly synthesized Schiff base ligand 2-hydroxy-3-((4-(4-phenylthiazol-2-yl) semicarbazide) methyl) benzoic acid behaves as tridentate OON donor and the complexes of square pyramidal coordination type [ML (Cl)2]. The help of various physicochemical and spectroscopic methods such as IR, ^{1}H NMR, the square pyramidal coordination geometries of Cu (II), Co (II), Ni (II), and Zn (II) complexes have been proposed. The non-electrolyte nature of the complexes was confirmed on the basis of their molar conductance values. The newly synthesized metal complexes having good antimicrobial activity when compared to Schiff base ligand. The DNA cleavage activity of all the newly synthesized compounds showed the cleavage of plasmid DNA cleavage. In addition to that, cytotoxicity of Co (II) and Zn (II) complexes indicate potent cytotoxic agents that might become potent anticancer agent in clinical trials. Hence from all these extensive observations; it was concluded that the Schiff base ligand (L) and its metal complexes give the significant, adaptable and valuable information of coordination compounds and also they may be used as potent biological agents with reduced toxicity and higher efficiency

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Cite this article: Karabasannavar SS, Allolli PR, Kalshetty BM. Synthesis, Characterization, Antimicrobial, DNA cleavage, and Cytotoxicity Studies of Some Metal (II) Complexes of tridentate Schiff Base Ligand: 2-hydroxy-3-((4-(4-phenylthiazol-2-yl) semicarbazide) methyl) benzoic acid. Indian J of Pharmaceutical Education and Research. 2017;51(4):748-57.

Indonesian Journal of Electrical Engineering and Informatics (IJEEI)
Vol. 5, No. 2, June 2017, pp. 155~161
ISSN: 2089-3272, DOI: 10.11591/ijeei.v5i2.258

Computing Some Degree-Based Topological Indices of Graphene

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Abstract

Graphene is one of the most promising nanomaterial because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and bio devices. Inspired by recent work on Graphene of computing topological indices, here we compute new topological indices viz. Arithmetic-Geometric index (AG2 index), SK3 index and Sanskruti index of a molecular graph G and obtain the explicit formulae of these indices for Graphene.

Keywords*: Arithmetic-Geometric index (AG2 index), SK3 index, sanskruti index, graphene.*

1. Introduction

A molecular graph is a representation of a chemical compound having atoms as vertices and the bonds between atoms correspond to the edge of the graph. The collection of vertices of a graph, says G, is denoted by V (G) and the set of edges is denoted by E (G). The degree of a vertex v of a graph is the number of vertices of G adjacent to v, denoted by dG (v) or simply as dv [3].

Molecular graphs are a special type of chemical graphs, which represent the constitution of molecules. They are also called constitutional graphs. When the constitutional graph of a molecule is represented in a two-dimentional basis it is called structural graphs [7, 8].

Topological invariant of a graph is a single number descriptor which is correlated to certain chemical, thermodynamical and biological behavior of the chemical compounds. Several topological indices have been defined over past decades which depend on degree of vertices.

2. Computing the Topological Indices of Graphene.

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industries worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Also it is the most effective material for electromagnetic interference (EMI) shielding. Now we focus on computation of topological indices of Graphene [1, 4].

Motivated by previous research on Graphene [4,6,11-14], here we compute three new topological indices viz. Arithmetic-Geometric index (AG2 index), SK3 index and Sanskruti index of a molecular graph G and obtain the explicit formulae of these indices for Graphene.

2.1. Arithmetic-Geometric (AG_2) Index

Let G = (V, E) be a molecular graph, and SG(u) is the degree of the vertex u, then AG2 index of G is defined as

$$AG2\ (G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u).S_G(v)}}$$

Received Oct 20, 2016; Revised April 21, 2017; Accepted May 12, 2017

where, AG2 index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where SG (u) (or SG (v)) is the summation of degrees of all neighbours of vertex u (or v) in G.

SG (u) = $\sum_{u,v\in E(G)} d_G(u)$ and NG (u) = {v∈V (G)/uv∈E (G)}

2.2. *SK$_3$* Index

The SK3 index of a graph G = (V, E) is defined as

SK3 (G) = $\sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2}$

where SG (u) (or SG (v)) is the summation of degrees of all neighbours of vertex u (or v) in G.

SG (u) = $\sum_{u,v\in E(G)} d_G(u)$ and NG (u) = {v∈V (G)/uv∈E (G)}

2.3. Sanskruti Index

Recently, Hosamani [9], studied a novel topological index, namely the Sanskruti index S (G) of a molecular graph G, which is denoted as

S (G) = $\sum_{uv\in E(G)} \left(\frac{S_G(u).S_G(v)}{S_G(u)+S_G(v)-2} \right)^3$

where SG (u) (or SG (v)) is the summation of degrees of all neighbours of vertex u (or v) in G.

SG (u) = $\sum_{u,v\in E(G)} d_G(u)$ and NG (u) = {v∈V (G)/uv∈E (G)}

3. Main Results

3.1. The *AG$_2$* index of Graphene is

$$AG_2\,(G) = \begin{cases} 6.0588t + 2.0277s + 3ts - 1.0032 & if\ t \neq 1 \\ 5.0119s + 1.0578 & if\ t = 1 \\ 6 & if\ t = 1, s > 1 \end{cases}$$

Let $e_{i,\,j}$ denote the number of edges with *i=Su* and *j=Sv*. It is easy to see that the summation of degrees of edge endpoints of Graphene has nine edge types $e_{4,5}$, $e_{5,5}$, $e_{5,7}$, $e_{5,8}$, $e_{6,7}$, $e_{7,9}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$ that are enumerated Table 1. For convenience these edge type are colored by grey, yellow, red, purple, blue, green, light blue, brown, and black, respectively, as shown in Figure 1.

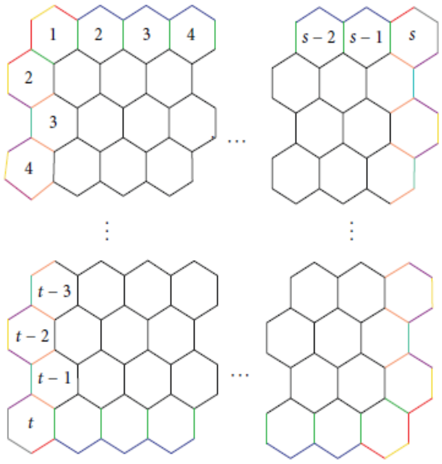

Figure 1. Colors of Graphene Edge (1)

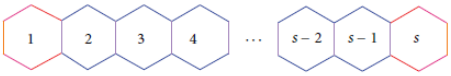

Figure 2. Colors of Graphene Edge (2)

Case 1. The AG_2 index of Graphene for t ≠1 is

$$AG_2\,(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2\sqrt{S_G(u).S_G(v)}}$$

Table 1. Nine edge types of Graphene

Rows	$e_{4,5}$	$e_{5,5}$	$e_{5,7}$	$e_{5,8}$	$e_{6,7}$	$e_{7,9}$	$e_{8,8}$	$e_{8,9}$	$e_{9,9}$
1	2	1	3	1	2s-4	s	0	1	2s-3
2	0	1	1	1	0	0	1	2	3s-4
3	0	1	0	2	0	0	1	2	3s-4
4	0	1	0	2	0	0	1	2	3s-4
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.
t-2	0	1	0	2	0	0	1	2	3s-4
t-1	0	1	1	1	0	0	1	1	3s-4
t	2	1	3	1	2s-4	s	0	0	0
Total	4	t	8	2t-4	4s-8	2s	t-2	2t-4	3ts-4s-4t+5

$$AG_2\,(G) = \left(e_{4,5}\right)\left(\frac{4+5}{2\sqrt{20}}\right)+\left(e_{5,5}\right)\left(\frac{5+5}{2\sqrt{25}}\right)+\left(e_{5,7}\right)\left(\frac{5+7}{2\sqrt{35}}\right)+\left(e_{5,8}\right)\left(\frac{5+8}{2\sqrt{40}}\right)+\left(e_{6,7}\right)$$

$$\left(\frac{6+7}{2\sqrt{42}}\right)\left(e_{7,9}\right)\left(\frac{7+9}{2\sqrt{63}}\right)+\left(e_{8,8}\right)\left(\frac{8+8}{2\sqrt{64}}\right)+\left(e_{9,8}\right)\left(\frac{9+8}{2\sqrt{72}}\right)+\left(e_{9,9}\right)\left(\frac{9+9}{2\sqrt{81}}\right)$$

$$= (4)\left(\frac{9}{2\sqrt{20}}\right)+(t)\left(\frac{10}{2\sqrt{25}}\right)+(8)\left(\frac{12}{2\sqrt{35}}\right)+(2t-4)\left(\frac{13}{2\sqrt{40}}\right)+(4s-8)\left(\frac{13}{2\sqrt{42}}\right)$$

$$+(2s)\left(\frac{16}{2\sqrt{63}}\right)+(t-2)\left(\frac{16}{2\sqrt{64}}\right)+(2t-4)\left(\frac{17}{2\sqrt{72}}\right)+(3ts-4s-4t+5)\left(\frac{18}{2\sqrt{81}}\right)$$

$$=\left(5+\frac{13}{\sqrt{40}}+1+\frac{17}{\sqrt{72}}-4\right)t+\left(\frac{26}{\sqrt{42}}+\frac{16}{\sqrt{63}}-4\right)s+3ts+$$
$$\left(\frac{18}{\sqrt{20}}+\frac{48}{\sqrt{35}}-\frac{26}{\sqrt{40}}-\frac{52}{\sqrt{42}}-2-\frac{34}{\sqrt{72}}+5\right)$$

$= 6.0588t + 2.0277s + 3ts - 1.0032$

Case 2. For *t=1* and *s>1*, Graphene has five types of edges, namely $e_{4,4}$, $e_{4,5}$, $e_{5,7}$, $e_{6,7}$, and $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 2. The number of edges of these types is shown in Table 2

Table 2. The Number of Edges

Number of benzene rings(s)	$e_{4,4}$	$e_{4,5}$	$e_{5,7}$	$e_{6,7}$	$e_{7,7}$
2	2	4	4	0	1
3	2	4	4	4	2
4	2	4	4	8	3
5	2	4	4	12	4
.	.	.	.	.	.
.	.	.	.	.	.
s-1	2	4	4	4s-12	s-2
s	2	4	4	4s-8	s-1

$$AG_2(G)=(e_{4,4})\left(\frac{4+4}{2\sqrt{16}}\right)+(e_{4,5})\left(\frac{4+5}{2\sqrt{20}}\right)+(e_{5,7})\left(\frac{5+7}{2\sqrt{35}}\right)+(e_{6,7})\left(\frac{6+7}{2\sqrt{42}}\right)+(e_{7,7})\left(\frac{7+7}{2\sqrt{49}}\right)$$

$$=(2)\left(\frac{8}{2\sqrt{16}}\right)+(4)\left(\frac{9}{2\sqrt{20}}\right)+(4)\left(\frac{12}{2\sqrt{35}}\right)+(4s-8)\left(\frac{13}{2\sqrt{40}}\right)+(s-1)\left(\frac{14}{2\sqrt{49}}\right)$$

$$=\left(2+\frac{18}{\sqrt{20}}+\frac{24}{\sqrt{35}}-\frac{52}{\sqrt{42}}-1\right)t+\left(\frac{26}{\sqrt{42}}+1\right)s$$

$= 5.0119s + 1.0578$

Case 3. For t=1 and s=1, we have only 6 edges of the type e4,4 as shown in Figure 3.

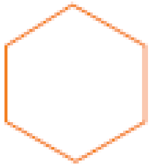

Figure 3. Type $e_{4,4}$ with 6 Edges

$$AG_2\,(G) = \left(e_{4,4}\right)\left(\frac{4+4}{2\sqrt{16}}\right)=6$$

3.2. The SK_3 index of Graphene is

$$SK_3\,(G) = \begin{cases} 7t+6s+27ts-17 & if\ t\neq 1 \\ 33s-9 & if\ t=1 \\ 24 & if\ t=1, s>1 \end{cases}$$

Proof: Let $e_{i,j}$ denote the number of edges with $i=Su$ and $j=Sv$. It is easy to see that the summation of degrees of edge endpoints of Graphene has nine edge types $e_{4,5}$, $e_{5,5}$, $e_{5,7}$, $e_{5,8}$, $e_{6,7}$, $e_{7,9}$, $e_{8,8}$, $e_{8,9}$ and $e_{9,9}$ that are enumerated Table1. For convenience these edge type are colored by grey, yellow, red, purple, blue, green, light blue, brown, and black, respectively, as shown in Figure1.

Case 1. The SK_3 index of Graphene for $t \neq 1$ is

$$SK_3\,(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2}$$

$$SK_3(G) = \left(e_{4,5}\right)\left(\frac{4+5}{2}\right)+\left(e_{5,5}\right)\left(\frac{5+5}{2}\right)+\left(e_{5,7}\right)\left(\frac{5+7}{2}\right)+\left(e_{5,8}\right)\left(\frac{5+8}{2}\right)+\left(e_{6,7}\right)\left(\frac{6+7}{2}\right)+$$

$$\left(e_{7,9}\right)\left(\frac{7+9}{2}\right)+\left(e_{8,8}\right)\left(\frac{8+8}{2}\right)+\left(e_{9,8}\right)\left(\frac{9+8}{2}\right)+\left(e_{9,9}\right)\left(\frac{9+9}{2}\right)$$

$$= (4)\left(\frac{9}{2}\right)+(t)\left(\frac{10}{2}\right)+(8)\left(\frac{12}{2}\right)+(2t-4)\left(\frac{13}{2}\right)+(4s-8)\left(\frac{13}{2}\right)+(2s)\left(\frac{16}{2}\right)+(t-2)$$

$$\left(\frac{16}{2}\right)+(2t-4)\left(\frac{17}{2}\right)+(3ts-4s-4t+5)\left(\frac{18}{2}\right)$$

$$=(5+13+8+17-36)t+(26+16-36)s+27ts+(18+48-26-52-16-34+45)$$

$$= 7t + 6s + 27ts - 17$$

Case 2. For $t=1$ and $s>1$, Graphene has five types of edges, namely $e_{4,4}$, $e_{4,5}$, $e_{5,7}$, $e_{6,7}$, and $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 2. The number of edges of these types is shown in Table 2.

$$SK_3\,(G) = \left(e_{4,4}\right)\left(\frac{4+4}{2}\right)+\left(e_{4,5}\right)\left(\frac{4+5}{2}\right)+\left(e_{5,7}\right)\left(\frac{5+7}{2}\right)+\left(e_{6,7}\right)\left(\frac{6+7}{2}\right)+\left(e_{7,7}\right)\left(\frac{7+7}{2}\right)$$

$$= (2)\left(\frac{8}{2}\right)+(4)\left(\frac{9}{2}\right)+(4)\left(\frac{12}{2}\right)+(4s-8)\left(\frac{13}{2}\right)+(s-1)\left(\frac{14}{2}\right)$$

$$= (8+18+24-52-7)t+(26+7)s$$

$$= 33s - 9$$

Case 3. For *t=1* and *s=1*, we have only 6 edges of the type $e_{4,4}$ as shown in Figure 3.

$$SK_3(G) = \left(e_{4,4}\right)\left(\frac{4+4}{2}\right) = 24$$

3.3. The Sanskruti index of Graphene is

$$S(G) = \begin{cases} 389.22ts - 75.58t - 114.06s - 186.08 & if\ t \neq 1 \\ 290.72s - 210.68 & if\ t = 1, s > 1 \\ 113.76 & if\ t = 1, s = 1 \end{cases}$$

Proof: Let $e_{i,j}$ denote the number of edges with *i=Su* and *j=Sv*. It is easy to see that the summation of degrees of edge endpoints of Graphene has nine edge types $e_{4,5}, e_{5,5}, e_{5,7}, e_{5,8}, e_{6,7}, e_{7,9}, e_{8,8}, e_{8,9}$ and $e_{9,9}$ that are enumerated Table 1. For convenience these edge type are colored by grey, yellow, red, purple, blue, green, light blue, brown, and black, respectively, as shown in Figure 1.

Case 1. The Sanskruti index of Graphene for *t ≠1* is

$$S(G) = \sum_{uv \in E(G)} \left(\frac{S_G(u).S_G(v)}{S_G(u)+S_G(v)-2} \right)^3$$

$$S(G) = \left(e_{4,5}\right)\left(\frac{4\times5}{4+5-2}\right)^3 + \left(e_{5,5}\right)\left(\frac{5\times5}{5+5-2}\right)^3 + \left(e_{5,7}\right)\left(\frac{5\times7}{5+7-2}\right)^3 + \left(e_{5,8}\right)\left(\frac{5\times8}{5+8-2}\right)^3 + \left(e_{6,7}\right)\left(\frac{6\times7}{6+7-2}\right)^3 + \left(e_{7,9}\right)\left(\frac{7\times9}{7+9-2}\right)^3 + \left(e_{8,8}\right)\left(\frac{8\times8}{8+8-2}\right)^3 + \left(e_{9,8}\right)\left(\frac{9\times8}{9+8-2}\right)^3 + \left(e_{9,9}\right)\left(\frac{9\times9}{9+9-2}\right)^3$$

$$= (4)\left(\frac{20}{7}\right)^3 + (t)\left(\frac{25}{8}\right)^3 + (8)\left(\frac{35}{10}\right)^3 + (2t-4)\left(\frac{40}{11}\right)^3 + (4s-8)\left(\frac{42}{11}\right)^3 + (2s)\left(\frac{63}{14}\right)^3 + (t-2)\left(\frac{64}{14}\right)^3 + (2t-4)\left(\frac{72}{15}\right)^3 + (3ts-4s-4t+5)\left(\frac{81}{16}\right)^3$$

$$= \left(\left(\frac{25}{8}\right)^3 + 2\left(\frac{40}{11}\right)^3 + \left(\frac{64}{14}\right)^3 + 2\left(\frac{72}{15}\right)^3 - 4\left(\frac{81}{16}\right)^3\right)t + \left(4\left(\frac{42}{11}\right)^3 + 2\left(\frac{63}{14}\right)^3 - 4\left(\frac{81}{16}\right)^3\right)s + 3ts\left(\frac{81}{16}\right)^3 + \left(4\left(\frac{20}{7}\right)^3 + 8\left(\frac{35}{10}\right)^3 - 4\left(\frac{40}{11}\right)^3 - 8\left(\frac{42}{11}\right)^3 - 2\left(\frac{64}{14}\right)^3 - 4\left(\frac{72}{15}\right)^3 + 5\left(\frac{81}{16}\right)^3\right)$$

$$= 389.22t\,s - 75.58t - 114.06s - 186.08$$

Case 2. For *t=1* and *s>1*, Graphene has five types of edges, namely $e_{4,4}, e_{4,5}, e_{5,7}, e_{6,7}$, and $e_{7,7}$. These edges are colored in orange, pink, red, blue, and lavender, respectively, as shown in Figure 2. The number of edges of these types is shown in Table 2.

$$S\,(G) = \left(e_{4,4}\right)\left(\frac{4\times4}{4+4-2}\right)^3+\left(e_{4,5}\right)\left(\frac{4\times5}{4+5-2}\right)^3+\left(e_{5,7}\right)\left(\frac{5\times7}{5+7-2}\right)^3+\left(e_{6,7}\right)\left(\frac{6\times7}{6+7-2}\right)^3+\left(e_{7,7}\right)\left(\frac{7\times7}{7+7-2}\right)^3$$

$$= (2)\left(\frac{16}{6}\right)^3+(4)\left(\frac{20}{7}\right)^3+(4)\left(\frac{35}{10}\right)^3+(4s-8)\left(\frac{42}{11}\right)^3+(s-1)\left(\frac{49}{12}\right)^3$$

$$=\left(4\left(\frac{42}{11}\right)^3+\left(\frac{49}{12}\right)^3\right)s+\left(2\left(\frac{16}{6}\right)^3+4\left(\frac{20}{7}\right)^3+4\left(\frac{35}{10}\right)^3-8\left(\frac{42}{11}\right)^3-1\left(\frac{49}{12}\right)^3\right)$$

$$= 290.72s - 210.68$$

Case 3. For *t=1* and *s=1*, we have only 6 edges of the type $e_{4,\,4}$ as shown in Figure 3

$$S\,(G) = \left(e_{4,4}\right)\left(\frac{4\times4}{4+4-2}\right)^3 = 113.76$$

4. Conclusion

In this paper we have computed the Arithmetic-Geometric (AG_2) index, SK_3 index and Sanskruti index $S\,(G)$ of Graphene is obtained without using computer.

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TWMS J. App. Eng. Math. V.8, N.2, 2018, pp. 477-482

COMPUTING SANSKRUTI INDEX OF CERTAIN NANOTUBES

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Abstract. Recently, Hosamani [8], has studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G. The Sanskruti index $S(G)$ shows good correlation with entropy of octane isomers. In this paper we compute the Sanskruti index $S(G)$ of $NHPX[m,n]$ and $TUC_4[m,n]$ nanotubes.

Keywords: Molecular graph, H-Naphtalenic nanotube, $TUC_4[m,n]$ nanotube, Sanskruti index.

AMS Subject Classification: 05C90

1. Introduction

A molecular graph is a representation of a chemical compound having atoms as vertices and the bonds between atoms correspond to the edge of the graph. The collection of vertices of a graph, say G, is denoted by $V(G)$ and the set of edges is denoted by $E(G)$. The degree of a vertex v of a graph is the number of vertices of G adjacent to v, denoted by $d_G(v)$ or simply as d_v[2,3,14].

Topological invariant of a graph is a single number descriptor which is correlated to certain chemical, thermo-dynamical and biological behavior of the chemical compounds. Several topological indices have been defined over past decades which depend on degree of vertices.

Historically, the first vertex-degree-based structure descriptors were the graph invariants that now a days are called Zagreb indices [4].

$$M_1(G) = \sum_{u \epsilon V(G))} (d_G(u))^2 \tag{1}$$

$$M_2(G) = \sum_{uv \epsilon E(G))} (d_G(u) d_G(v)) \tag{2}$$

However,initially these were intended to be used for a completely different purpose and these were included among topological indices much later. The first genuine degree-based topological index was put-forward in 1975 by Milan Randić in his seminar paper on

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§ Manuscript received: January 3, 2017; accepted: February 3, 2017.

characterization of molecular branching [9] his index was defined as

$$R(G) = \sum_{uv \epsilon E(G))} \frac{1}{\sqrt{d_G(u) d_G(v)}} \tag{3}$$

Recently, Hosamani [8], studied a novel topological index, namely the Sanskruti index $S(G)$ of a molecular graph G.

$$S(G) = \sum_{uv \epsilon E(G))} \left(\frac{S_G(u) S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3 \tag{4}$$

where $S_G(u)$ and $S_G(v)$ is the summation of degrees of all neighbours of vertices u and v in G.

$$S_G(u) = \sum_{u,v \epsilon E(G)} d_G(u)$$

and

$$N_G(u) = v \epsilon V(G)/uv \epsilon E(G)$$

The Sanskruti index shows good correlation with the entropy of octane isomers which is depicted in Figure 1.

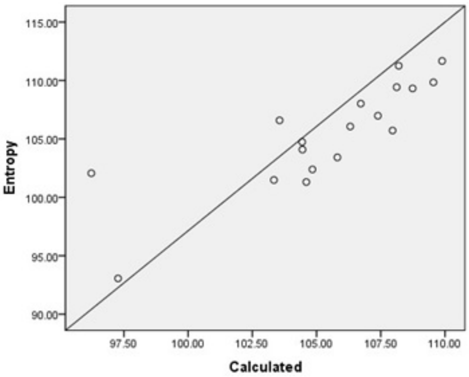

FIGURE 1. Correlations of S with entropy of octane isomers ($entropy = 1.7857S \pm 81.4286$).

In this paper, we continue the process of computing the Sanskruti index of some more nanotubes, which are $NHPX[m,n]$ and $TUC_4[m,n]$ nanotubes[1,6,7,10,11,12].

2. MAIN RESULTS AND DISSECTION

2.1. **H-Naphtalenic Nanotube.** In this section, we compute the certainC_6, C_6, C_4, C_6, C_6, C_4 in first row and a sequence of C_6,C_8, C_6, C_8 in other row. In other words, the whole lattice is a plane tiling can either cover a cylinder or a torus. These nanotube usually symbolized as $NPHX[m,n]$, in which m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as depicted in Figure 2. Now

TABLE 1. Edge partition of graph of $NHPX[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_a, S_b) where $u,v \epsilon E(H)$	(6,7)	(6,8)	(8,8)	(7,9)	(8,9)	(9,9)
Number of edges	$4m$	$4m$	$2m$	$2m$	$4m$	$15mn - 18m$

we compute important topological index Sanskruti index for 2D-lattice of $NHPX[m,n]$ nanotube. There are six types of edges in $NHPX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge as depicted in Figure 2 , in which different colours shows different partite sets of edge set of $NHPX[m,n]$ nanotube. In Figure 2, red colour shows the edges ab with $S_a = 6$ and $S_b = 7$, blue colour shows the type of edges ab with $S_a = 6$ and $S_b = 8$, green colour shows the type of edges ab with $S_a = S_b = 8$, yellow colour shows the type of edges ab with $S_a = 7$ and $S_b = 9$, brown colour shows the type of edges ab with $S_a = 8$ and $S_b = 9$ and black colour shows the partition having edges ab with $S_a = S_b = 9$.

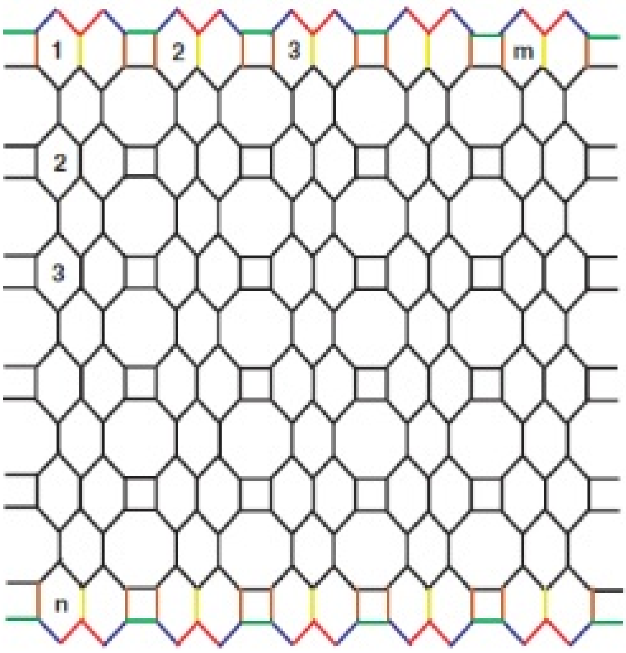

FIGURE 2. A graph of H-Naphtalenic nanotube $NPHX[m,n]$ showing different partite sets based on the degree sum of neighbors of end vertices of each edge.

In Table 1, cardinalities of such partite sets of edge set of graph of $NHPX[m,n]$ nanotube are shown. In the following theorem Sanskruti index of $NHPX[m,n]$ nanotube is computed.

Theorem 2.1. *Consider the graph of $NPHX[m,n]$ nanotubes, then its Sanskruti index is equal to*

$$S(NPHX[m,n]) = (1945.61n - 928.152)m$$

Proof. We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge.
NOW by using the partition given in Table1 we can apply the formula of Sanskruti index to compute this index for $NPHX[m,n]$ nanotube.

$$S(G) = \sum_{uv\epsilon E(G))} \left(\frac{S_G(u)S_G(v)}{S_G(u) + S_G(v) - 2} \right)^3$$

$$\begin{aligned}
AG_2(NPHX(n)) &= (e_{6,7})\left(\frac{6\times 7}{6+7-2}\right)^3+(e_{6,8})\left(\frac{6\times 8}{6+8-2}\right)^3+(e_{8,8})\left(\frac{8\times 8}{8+8-2}\right)^3\\
&+ (e_{7,9})\left(\frac{7\times 9}{7+9-2}\right)^3+(e_{8,9})\left(\frac{8\times 9}{8+9-2}\right)^3+(e_{9,9})\left(\frac{9\times 9}{9+9-2}\right)^3\\
&= 4m\left(\frac{6\times 7}{6+7-2}\right)^3+4m\left(\frac{6\times 8}{6+8-2}\right)^3+2m\left(\frac{8\times 8}{8+8-2}\right)^3+2m\left(\frac{7\times 9}{7+9-2}\right)^3\\
&+ 4m\left(\frac{8\times 9}{8+9-2}\right)^3+(15mn-8m)\left(\frac{9\times 9}{9+9-2}\right)^3\\
&= 4m\left(\frac{42}{11}\right)^3+4m\left(\frac{48}{12}\right)^3+2m\left(\frac{64}{14}\right)^3+2m\left(\frac{63}{14}\right)^3+4m\left(\frac{72}{15}\right)^3\\
&+ (15mn-8m)\left(\frac{81}{16}\right)^3\\
&= \left(4\left(\frac{42}{11}\right)^3+4\left(\frac{48}{12}\right)^3+2\left(\frac{64}{14}\right)^3+2\left(\frac{63}{14}\right)^3+4\left(\frac{72}{15}\right)^3-18\left(\frac{81}{16}\right)^3\right)m\\
&+ \left(15\left(\frac{81}{16}\right)^3\right)mn\\
&= (1945.61n-928.152)m
\end{aligned}$$

2.2. **Nanotube Covered by C_4.** In this section, we compute certain topological indices of nanotube covered only by C_4. The 2D-lattice of this family of nanotube is a plane tiling of C_4. This tessellation of C_4 can either cover a cylinder or a torus. This family of nanotube is denoted by $TUC_4[m,n]$, in which m is the number of squares in a row and n is the number of squares in a column as shown in Figure 3.

Now we compute Sanskruti index for two dimensional lattice of $TUC_4[m,n]$ nanotube. There are five types of edges in the graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each as shown in Figure 3 in which red coloured edges are the edge ab with $S_a=S_b=7$, blue coloured edges are the edge ab with $S_a=7$ and $S_b=15$, green coloured edges are the edge ab with $S_a=S_b=15$, yellow coloured edges are the edge ab with $S_a=15$ and $S_b=16$, black coloured edges are the edge ab with $S_a=S_b=16$. Table2 shows the cardinalities of these partite sets.

TABLE 2. Edge partition of graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

$(S_a,\ S_b)$ where $u,v\epsilon E(H)$	(7,7)	(7,15)	(15,15)	(15,16)	(16,16)
Number of edges	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(m+1)(2n-7)$

Theorem 2.2. *Let the graph of $TUC_4[m,n]$ nanotube with $(m\geq 1, n\geq 4)$, then its Sanskruti index is*

$$S(TUC_4[m,n])=(1242.74n-1752.65)(m+1)$$

Proof. We use the edge partition of graph of $TUC_4[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge.
Now by using the partition given in Table2 we can apply the formula of index to compute this index for $TUC_4[m,n]$ nanotube.

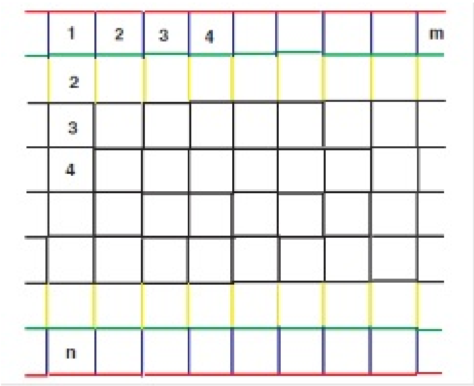

FIGURE 3. A graph of $TUC_4[m,n]$ nanotube showing the edge partition based on the degree sum of end vertices lying at unit distance from end vertices of each edge.

$$S(G) = \sum_{uv\epsilon E(G))} \left(\frac{S_G(u)S_G(v)}{S_G(u)+S_G(v)-2} \right)^3$$

$$\begin{aligned}
S(TUC_4[m,n]) &= (e_{7,7}) \left(\frac{7\times 7}{7+7-2} \right)^3 + (e_{7,15}) \left(\frac{7\times 15}{7+15-2} \right)^3 \\
&+ (e_{15,15}) \left(\frac{15\times 15}{15+15-2} \right)^3 + (e_{15,16}) \left(\frac{15\times 16}{15+16-2} \right)^3 + (e_{16,16}) \left(\frac{16\times 16}{16+16-2} \right)^3 \\
&= (2m+2) \left(\frac{7\times 7}{7+7-2} \right)^3 + (2m+2) \left(\frac{7\times 15}{7+15-2} \right)^3 \\
&+ (2m+2) \left(\frac{15\times 15}{15+15-2} \right)^3 + (2m+2) \left(\frac{15\times 16}{15+16-2} \right)^3 \\
&+ (m+1)(2n-7) \left(\frac{16\times 16}{16+16-2} \right)^3 \\
&= (2m+2) \left(\frac{49}{12} \right)^3 + (2m+2) \left(\frac{105}{20} \right)^3 + (2m+2) \left(\frac{225}{28} \right)^3 + (2m+2) \left(\frac{240}{29} \right)^3 \\
&+ (m+1)(2n-7) \left(\frac{256}{30} \right)^3 \\
&= \left(2\left(\frac{49}{12} \right)^3 + 2\left(\frac{105}{20} \right)^3 + 2\left(\frac{225}{28} \right)^3 + 2\left(\frac{240}{29} \right)^3 - 7\left(\frac{256}{30} \right)^3 \right) m \\
&+ \left(\frac{256}{30} \right)^3 2mn + \left(\frac{240}{29} \right)^3 2n \\
&+ \left(2\left(\frac{49}{12} \right)^3 + 2\left(\frac{105}{20} \right)^3 + 2\left(\frac{225}{28} \right)^3 + 2\left(\frac{240}{29} \right)^3 - 7\left(\frac{256}{30} \right)^3 \right) \\
&= (1242.74n - 1752.65)(m+1)
\end{aligned}$$

3. Conclusion

In this paper, we have computed the value of Sanskruti index for H-Naphtalenic nanotube and $TUC_4[m, n]$ nanotube without using computer.

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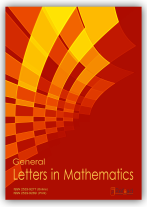
Available online at www.refaad.com
Gen.Lett. Math., 9(1) (2020), 9-16
Research Article

General Letters in Mathematics (GLM)
Journal Homepage: http://www.refaad.com/views/GLM/home.aspx
ISSN: 2519-9277 (Online) 2519-9269 (Print)



QSPR Analysis of Chemical Graph Theory

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Abstract

In this paper, we find the values of four important degree-based topological indices of molecular graph of alkane isomers. Further, we show that these parameters are highly correlated with physical properties of alkane isomers. . ©2019 All rights reserved.

Keywords: Alkane isomers,, Degree-based topological indices.
2010 MSC: 05C10, 57M15, 57M25.

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1. Introduction

Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \epsilon V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [4].

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. Hence chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. It has found to be a useful tool in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) [8, 5, 14]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices. In 1975, Randic [10] proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [4, 2, 11]. This theory had an important effect on the development of the chemical sciences.

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doi:10.31559/glm2020.9.1.2

Received 6 Jul 2018 : Accepted 12 Aug 2020

2. Computing Some New Degree-Based Topological Indices

We consider the following most studied degree based topological indices for QSPR study [12, 14, 15, 16].

Definition 2.1. Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u, then Arithmetic-Geometric Index $(AG_1 index)$ of G is defined as

$$AG_1(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}$$

Where, $(AG_1 index)$ is considered for distinct vertices.
The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ $(or\ d_G(v))$ denotes the degree of the vertex $u\,(or\ v)$.

Definition 2.2. The SK index of a graph $G = (V, E)$ is defined as $SK(G)=\sum_{u,v\epsilon E(G)}^{\cdot} \frac{d_G(u)+d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.3. The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G)=\sum_{u,v\epsilon E(G)}^{\cdot} \frac{d_G(u).d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.4. The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G)=\sum_{u,v\epsilon E(G)}^{\cdot} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Motivation

By looking at the earlier results QSPR Analysis of Certain Degree-Based Topological Indices and QSPR Analysis of Degree-Based Topological Indices with physical properties of Benzenoid Hydrocarbons [7, 5, 6, 13].

3. Data Sources and Analytical Method

Energy of Alkane isomers are taken from [19, 7, 12, 5]. Seven physicochemical properties of Alkane isomers have been selected on the availability of a suitable body of data: *boiling point* (BP), *critical temperature* (CT), *critical pressure* (CP), *Molar volume* (CV), *Molar refraction* (MR), *Heat of Vaporization* (HV), *Surface tension* (ST). The values are compiled in Table 2.

4. Results and Discussion

In Table 3, the correlation coefficient of topological indices with physicochemical properties of alkane isomers are found to be good.

4.1. Regression Models

We have tested the following linear regression model

$$P = a + b\,(TI) \tag{4.1}$$

where, P=Physical property, TI=Topological Index. Using (4.1), we have obtained the following different linear models for each degree-based topological index, which are listed below.

Table 1: The topological indices (AG1 Index, SK Index, SK1 Index and SK2 Index) values of Alkane Isomers.

S.NO.	Compound Name	AG1 Index	SK Index	SK1 Index	SK2 Index
1	Butane	3.1213	5	4	8.5
2	2-methyl propane	3.46410	6	4.5	12
3	Pentane	4.123	7	6	12.5
4	2-methyl butane	4.3906	8	7	16.5
5	2,2 dimethyl propane	5	10	8	25
6	Hexane	5.1213	9	8	16.5
7	2-methyl pentane	5.2359	10	9	20.5
8	3- methyl pentane	5.3172	10	9.5	21
9	2,2-dimethyl butane	5.8713	12	11	30
10	2,3- dimethyl butane	5.6188	11	10.5	25
11	Heptanes	6.1213	11	10	20.5
12	2-methyl hexane	6.3906	12	11	24.5
13	3- methyl hexane	6.5767	12	11.5	25
14	3-ethylpentane	6.2438	12	12	25.5
15	2,2-dimethyl pentane	6.8713	14	13	34
16	2,3- dimethyl pentane	6.54530	13	13	29.5
17	2,4- dimethyl pentane	6.6600	13	12	28.5
18	3,3- dimethyl pentane	6.7426	14	14	35
19	Octane	7.1213	13	12	24.5
20	2-methylheptane	7.3906	14	13	28.5
21	3- methylheptane	7.3172	14	13.5	29
22	4- methylheptane	7.3172	14	13.5	29
23	3-ethylhexane	7.2438	14	14	29.5
24	2,2-dimethylhexane	7.8713	16	15	38
25	2,3- dimethylhexane	7.5453	15	15	33.5
26	2,4- dimethylhexane	7.5866	15	14.5	33
27	2,5- dimethylhexane	7.6600	15	14	32.5
28	3,3- dimethylhexane	7.7426	16	16	39
29	3,4- dimethylhexane	7.4719	15	15.5	34
30	3-ethyl-2-methylpentane	7.4719	15	15.5	34
31	3-ethyl-3-methylpentane	7.6139	16	17	40
32	2,2,3-trimethylpentane	7.9963	17	17.5	43.5
33	2,2,4- trimethylpentane	8.1406	17	16	42
34	2,3,3- trimethylpentane	7.9410	17	18	44
35	2,3,4- trimethylpentane	8.4401	16	16.5	38
36	Nonane	8.1213	15	14	28.5
37	2-methyloctane	8.3906	16	15	32.5
38	3-methyloctane	8.3172	16	15.5	33
39	4-methyloctane	8.3172	16	15.5	33
40	3-ethylheptane	8.2438	16	16	33.5
41	4- ethylheptane	8.2438	16	16	33.5
42	2,2-dimethylheptane	8.8713	18	17	42
43	2,3- dimethylheptane	8.5453	17	17	37.5
44	2,4- dimethylheptane	10.8960	17	16.5	37
45	2,5- dimethylheptane	8.5866	17	16.5	37
46	2,6- dimethylheptane	8.6600	17	16	36.5
47	3,3- dimethylheptane	8.7426	18	18	43
48	3,4- dimethylheptane	7.4719	17	17.5	38
49	3,5- dimethylheptane	8.5132	17	17	37.5
50	4,4- dimethylheptane	8.7426	18	18	43
51	3-ethyl-2-methylhexane	8.4719	17	17.5	38
52	4-ethyl-2-methylhexane	8.5132	17	17	37.5
53	3-ethyl-3-methylhexane	7.0229	18	19	44
54	2,2,4-trimethylhexane	9.0672	19	18.5	46.5
55	2,2,5- trimethylhexane	9.1406	19	18	46
56	2,3,3- trimethylhexane	8.9410	19	20	48
57	2,3,4- trimethylhexane	8.7000	18	19	42.6
58	2,3,5- trimethylhexane	8.8147	18	18	41.5
59	3,3,4- trimethylhexane	8.8676	19	20.5	48.5
60	3,3-diethylpentane	8.4852	18	20	40.5
61	2,2-dimethyl-3-ethylpentane	8.9229	19	20	44.75
62	2,3-dimethyl-3ethylpentane	8.8124	19	21	49
63	2,4-dimethyl-3-ethylpentane	8.7000	18	19	42.5
64	2,2,3,3-tetramethylpentane	9.3713	21	23	58.5
65	2,2,3,4- tetramethylpentane	9.2244	20	21	52
66	2,2,4,4- tetramethylpentane	9.6213	21	20	55.5
67	2,3,3,4- tetramethylpentane	9.1395	20	22	53

1. AG_1 Index $(AG_1(G))$

$$Bp = 3.992 + 0.033AG_1(G) \tag{4.2}$$

$$CT = -0.976 + 0.03AG_1(G) \tag{4.3}$$

$$CP = 18.622 - 0.414AG_1(G) \tag{4.4}$$

$$MV = -3.525 + 0.069AG_1(G) \tag{4.5}$$

$$ST = -2.608 + 0.495AG_1(G) \tag{4.6}$$

Table 2: The physical and chemical properties (BP, MV, MR, HV, CT, CP, ST) of Alkane Isomers.

S.NO.	Compound Name	Bp(0C)	mv(cm3)	mr(cm3)	hv(kJ)	ct(0C)	cp(atm)	St(dyne/cm)
1	Butane	-0.500		20.68	22.44	152.01	37.47	12.46
2	2-methyl propane	-11.730		20.85	21.6	134.98	36	14.1
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00
5	2,2 dimethyl propane	9.503	112.074	25.7243	21.78	160.60	31.57	12.05
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42
7	2-methyl pentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38
8	3- methyl pentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12
9	2,2-dimethyl butane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30
10	2,3- dimethyl butane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26
12	2-methyl hexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29
13	3- methyl hexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44
15	2,2-dimethyl pentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02
16	2,3- dimethyl pentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96
17	2,4- dimethyl pentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15
18	3,3- dimethyl pentane	86.064	144.530	34.3323	33.02	263.00	30	19.59
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60
21	3- methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17
22	4- methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60
25	2,3- dimethylhexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99
26	2,4- dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05
27	2,5- dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73
28	3,3- dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63
29	3,4- dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67
33	2,2,4- trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77
34	2,3,3- trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56
35	2,3,4- trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81
41	4- ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80
43	2,3- dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34
44	2,4- dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30
45	2,5- dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30
46	2,6- dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83
47	3,3- dimethylheptane	137.00	176.897	43.6870	42.66	314.00	24.19	22.01
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22
54	2,2,4-trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31

Table 3: Correlation of topological indices with physicochemical properties of Alkane isomers.

	$Bp\left(^0\right)$	$ct\left(^0C\right)$	$cp\left(atm\right)$	$mv\left(cm^3\right)$	$st\left(\frac{dyne}{cm}\right)$	$hv\left(kJ\right)$	$mr\left(cm^3\right)$
AG_1	0.8463	0.8946	-0.8514	0.9186	0.8308	0.8614	0.9467
SK	0.8211	0.8945	-0.7661	0.8736	0.8097	0.8176	0.927
SK_1	0.8112	0.8959	-0.6730	0.8047	0.8290	0.7910	0.8864
SK_2	0.6841	0.7784	-0.5897	0.8047	0.6870	0.6522	0.7987

$$HV = -0.7 + 0.216 AG_1(G) \tag{4.7}$$

$$MR = -1.586 + 0.236 AG_1(G) \tag{4.8}$$

2. SK Index

$$Bp = 7.116 + 0.074 SK(G) \tag{4.9}$$

$$CT = -4.689 + 0.069 SK(G) \tag{4.10}$$

$$CP = 38.327 - 0.867 SK(G) \tag{4.11}$$

$$MV = -9.553 + 0.155 SK(G) \tag{4.12}$$

$$ST = -7.885 + 1.122 SK(G) \tag{4.13}$$

$$HV = -3.07 + 0.478 SK(G) \tag{4.14}$$

$$MR = -5.664 + 0.538 SK(G) \tag{4.15}$$

3. SK_1 Index

$$Bp = 5.565 + 0.087 SK_1(G) \tag{4.16}$$

$$CT = -8.611 + 0.083 SK_1(G) \tag{4.17}$$

$$CP = 39.199 - 0.905 SK_1(G) \tag{4.18}$$

$$MV = -12.542 + 0.172 SK_1(G) \tag{4.19}$$

$$ST = -13.031 + 1.365 SK_1(G) \tag{4.20}$$

$$HV = -5.945 + 0.549 SK_1(G) \tag{4.21}$$

$$MR = -8.648 + 0.611 SK_1(G) \tag{4.22}$$

4. SK_2 Index

$$Bp = 15.014 + 0.182 SK_2(G) \tag{4.23}$$

$$CT = -16.102 + 0.178 SK_2(G) \tag{4.24}$$

$$CP = 87.24 - 1.965 SK_2(G) \tag{4.25}$$

$$MV = -12.542 + 0.172 SK_2(G) \tag{4.26}$$

$$ST = -22.813 + 2.802 SK_2(G) \tag{4.27}$$

$$HV = -8.052 + 1.122 SK_2(G) \tag{4.28}$$

$$MR = -18.07 + 1.364 SK_2(G) \tag{4.29}$$

By inspection of the data in Table 4 to Table 7, it is possible to draw a number of conclusions for the given topological indices like invariants.

The QSPR study of $AG_1(G)$ index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 4, one can easily verify that $AG_1(G)$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $AG_1(G)$ index with physical properties of alkane isomers lies between -0.8514 to 0.9467.

Further, the correlation coefficient value of $AG_1(G)$ index is very high for the MR of alkane isomers with r =0.9467.Thus the QSPR study reveals that the $AG_1(G)$ index is an useful tool in predicting the

Table 4: Statistical parameters for the linear QSPR model for $AG_1(G)$.

Physical Properties	N	a	b	r
Boiling point	67	3.992	0.033	0.8463
Critical temperature	67	-0.976	0.03	0.8946
Critical pressure	67	18.622	-0.414	-0.8514
Molar volume	65	-3.525	0.069	0.9186
ST	67	-2.608	0.495	0.8308
HV	67	-0.7	0.216	0.8614
MR	67	-1.586	0.236	0.9467

Table 5: Statistical parameters for the linear QSPR model for $SK(G)$.

Physical Properties	N	a	b	r
Boiling point	67	7.116	0.074	0.8211
Critical temperature	67	-4.689	0.069	0.8945
Critical pressure	67	38.327	-0.867	-0.7661
Molar volume	65	-9.553	0.155	0.8736
ST	67	-7.885	1.122	0.8097
HV	67	-3.07	0.478	0.8176
MR	67	-5.664	0.538	0.927

Table 6: Statistical parameters for the linear QSPR model for $SK_1(G)$.

Physical Properties	N	a	b	r
Boiling point	67	5.565	0.087	0.8112
Critical temperature	67	-8.611	0.083	0.8959
Critical pressure	67	39.199	-0.905	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-13.031	1.365	0.829
HV	67	-5.945	0.549	0.791
MR	67	-8.648	0.611	0.8864

Table 7: Statistical parameters for the linear QSPR model for $SK_2(G)$.

Physical Properties	N	a	b	r
Boiling point	67	15.014	0.182	0.6841
Critical temperature	67	-16.102	0.178	0.7784
Critical pressure	67	87.24	-1.965	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-22.813	2.802	0.687
HV	67	-8.052	1.122	0.6522
MR	67	-18.07	1.364	0.7987

physical properties of alkane isomers. The QSPR study of $SK(G)\,index$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 5, one can easily verify that $SK(G)\,index$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK(G)\,\mathtt{index}$ with physical properties of alkane isomers lies between -0.7661 to 0.927. Further, the correlation coefficient value of $SK(G)\,\mathtt{index}$ index is very high for the MR of alkane isomers with r =0.927.Thus the QSPR study reveals that the $SK(G)\,\mathtt{index}$ index is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of $SK_1(G)\,\mathtt{index}$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 6, one can easily verify that $SK_1(G)\,\mathtt{index}$ shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK_1(G)\,\mathtt{index}$ with physical properties of alkane isomers lies between -0.673 to 0.8959. Further, the correlation coefficient value of $SK_1\mathtt{index}$ is very high for the CT of alkane isomers with r =0.8959.Thus the QSPR study reveals that the $SK_1(G)\,\mathtt{index}$ is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of $SK_2(G)\,\mathtt{index}$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 7, one can easily verify that $SK_2(G)\,\mathtt{index}$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK_2(G)\,\mathtt{index}$ with physical properties of alkane isomers lies between -0.673 to 0.7987. Further, the correlation coefficient value of $SK_2(G)\,\mathtt{index}$ is very high for the MR of alkane isomers with r =0.7987.Thus the QSPR study reveals that the $SK_2(G)\,\mathtt{index}$ is an useful tool in predicting the physical properties of alkane isomers.

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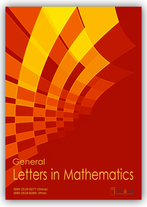
Available online at www.refaad.com
Gen.Lett. Math., 9(1) (2020), 9-16
Research Article

General Letters in Mathematics (GLM)
Journal Homepage: http://www.refaad.com/views/GLM/home.aspx
ISSN: 2519-9277 (Online) 2519-9269 (Print)



QSPR Analysis of Chemical Graph Theory

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Abstract

In this paper, we find the values of four important degree-based topological indices of molecular graph of alkane isomers. Further, we show that these parameters are highly correlated with physical properties of alkane isomers. . ©2019 All rights reserved.

Keywords: Alkane isomers,, Degree-based topological indices.
2010 MSC: 05C10, 57M15, 57M25.

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1. Introduction

Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \epsilon V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [4].

Chemical graph theory is the branch of mathematical chemistry. It is concerned with handling chemical graphs that represent chemical system. Hence chemical graph theory deals with analysis of all consequences of connectivity in a chemical system. It has found to be a useful tool in QSAR (Quantitative Structure-Activity Relationship) and QSPR (Quantitative Structure-Property Relationship) [8, 5, 14]. Numerous studies have been made relating to the above mentioned fields by using what are called topological indices. In 1975, Randic [10] proposed a topological index that has become one of the most widely used in both QSAR and QSPR studies.

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [4, 2, 11]. This theory had an important effect on the development of the chemical sciences.

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doi:10.31559/glm2020.9.1.2

Received 6 Jul 2018 : Accepted 12 Aug 2020

2. Computing Some New Degree-Based Topological Indices

We consider the following most studied degree based topological indices for QSPR study [12, 14, 15, 16].

Definition 2.1. Let $G = (V, E)$ be a molecular graph, and $d_G(u)$ is the degree of the vertex u, then Arithmetic-Geometric Index $(AG_1 index)$ of G is defined as

$$AG_1(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) . d_G(v)}}$$

Where, $(AG_1 index)$ is considered for distinct vertices.
The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ $(or\ d_G(v))$ denotes the degree of the vertex $u\,(or\ v)$.

Definition 2.2. The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u)+d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.3. The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \frac{d_G(u).d_G(v)}{2}$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Definition 2.4. The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v \epsilon E(G)}^{\cdot} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

Motivation

By looking at the earlier results QSPR Analysis of Certain Degree-Based Topological Indices and QSPR Analysis of Degree-Based Topological Indices with physical properties of Benzenoid Hydrocarbons [7, 5, 6, 13].

3. Data Sources and Analytical Method

Energy of Alkane isomers are taken from [19, 7, 12, 5]. Seven physicochemical properties of Alkane isomers have been selected on the availability of a suitable body of data: *boiling point* (BP), *critical temperature* (CT), *critical pressure* (CP), *Molar volume* (CV), *Molar refraction* (MR), *Heat of Vaporization* (HV), *Surface tension* (ST). The values are compiled in Table 2.

4. Results and Discussion

In Table 3, the correlation coefficient of topological indices with physicochemical properties of alkane isomers are found to be good.

4.1. *Regression Models*

We have tested the following linear regression model

$$P = a + b\,(TI) \tag{4.1}$$

where, P=Physical property, TI=Topological Index. Using (4.1), we have obtained the following different linear models for each degree-based topological index, which are listed below.

Table 1: The topological indices (AG1 Index, SK Index, SK1 Index and SK2 Index) values of Alkane Isomers.

S.NO.	Compound Name	AG1 Index	SK Index	SK1 Index	SK2 Index
1	Butane	3.1213	5	4	8.5
2	2-methyl propane	3.46410	6	4.5	12
3	Pentane	4.123	7	6	12.5
4	2-methyl butane	4.3906	8	7	16.5
5	2,2 dimethyl propane	5	10	8	25
6	Hexane	5.1213	9	8	16.5
7	2-methyl pentane	5.2359	10	9	20.5
8	3- methyl pentane	5.3172	10	9.5	21
9	2,2-dimethyl butane	5.8713	12	11	30
10	2,3- dimethyl butane	5.6188	11	10.5	25
11	Heptanes	6.1213	11	10	20.5
12	2-methyl hexane	6.3906	12	11	24.5
13	3- methyl hexane	6.5767	12	11.5	25
14	3-ethylpentane	6.2438	12	12	25.5
15	2,2-dimethyl pentane	6.8713	14	13	34
16	2,3- dimethyl pentane	6.54530	13	13	29.5
17	2,4- dimethyl pentane	6.6600	13	12	28.5
18	3,3- dimethyl pentane	6.7426	14	14	35
19	Octane	7.1213	13	12	24.5
20	2-methylheptane	7.3906	14	13	28.5
21	3- methylheptane	7.3172	14	13.5	29
22	4- methylheptane	7.3172	14	13.5	29
23	3-ethylhexane	7.2438	14	14	29.5
24	2,2-dimethylhexane	7.8713	16	15	38
25	2,3- dimethylhexane	7.5453	15	15	33.5
26	2,4- dimethylhexane	7.5866	15	14.5	33
27	2,5- dimethylhexane	7.6600	15	14	32.5
28	3,3- dimethylhexane	7.7426	16	16	39
29	3,4- dimethylhexane	7.4719	15	15.5	34
30	3-ethyl-2-methylpentane	7.4719	15	15.5	34
31	3-ethyl-3-methylpentane	7.6139	16	17	40
32	2,2,3-trimethylpentane	7.9963	17	17.5	43.5
33	2,2,4- trimethylpentane	8.1406	17	16	42
34	2,3,3- trimethylpentane	7.9410	17	18	44
35	2,3,4- trimethylpentane	8.4401	16	16.5	38
36	Nonane	8.1213	15	14	28.5
37	2-methyloctane	8.3906	16	15	32.5
38	3-methyloctane	8.3172	16	15.5	33
39	4-methyloctane	8.3172	16	15.5	33
40	3-ethylheptane	8.2438	16	16	33.5
41	4- ethylheptane	8.2438	16	16	33.5
42	2,2-dimethylheptane	8.8713	18	17	42
43	2,3- dimethylheptane	8.5453	17	17	37.5
44	2,4- dimethylheptane	10.8960	17	16.5	37
45	2,5- dimethylheptane	8.5866	17	16.5	37
46	2,6- dimethylheptane	8.6600	17	16	36.5
47	3,3- dimethylheptane	8.7426	18	18	43
48	3,4- dimethylheptane	7.4719	17	17.5	38
49	3,5- dimethylheptane	8.5132	17	17	37.5
50	4,4- dimethylheptane	8.7426	18	18	43
51	3-ethyl-2-methylhexane	8.4719	17	17.5	38
52	4-ethyl-2-methylhexane	8.5132	17	17	37.5
53	3-ethyl-3-methylhexane	7.0229	18	19	44
54	2,2,4-trimethylhexane	9.0672	19	18.5	46.5
55	2,2,5- trimethylhexane	9.1406	19	18	46
56	2,3,3- trimethylhexane	8.9410	19	20	48
57	2,3,4- trimethylhexane	8.7000	18	19	42.6
58	2,3,5- trimethylhexane	8.8147	18	18	41.5
59	3,3,4- trimethylhexane	8.8676	19	20.5	48.5
60	3,3-diethylpentane	8.4852	18	20	40.5
61	2,2-dimethyl-3-ethylpentane	8.9229	19	20	44.75
62	2,3-dimethyl-3ethylpentane	8.8124	19	21	49
63	2,4-dimethyl-3-ethylpentane	8.7000	18	19	42.5
64	2,2,3,3-tetramethylpentane	9.3713	21	23	58.5
65	2,2,3,4- tetramethylpentane	9.2244	20	21	52
66	2,2,4,4- tetramethylpentane	9.6213	21	20	55.5
67	2,3,3,4- tetramethylpentane	9.1395	20	22	53

1. AG_1 Index $(AG_1(G))$

$$Bp = 3.992 + 0.033AG_1(G) \tag{4.2}$$

$$CT = -0.976 + 0.03AG_1(G) \tag{4.3}$$

$$CP = 18.622 - 0.414AG_1(G) \tag{4.4}$$

$$MV = -3.525 + 0.069AG_1(G) \tag{4.5}$$

$$ST = -2.608 + 0.495AG_1(G) \tag{4.6}$$

Table 2: The physical and chemical properties (BP, MV, MR, HV, CT, CP, ST) of Alkane Isomers.

S.NO.	Compound Name	Bp(0C)	mv(cm3)	mr(cm3)	hv(kJ)	ct(0C)	cp(atm)	St(dyne/cm)
1	Butane	-0.500		20.68	22.44	152.01	37.47	12.46
2	2-methyl propane	-11.730		20.85	21.6	134.98	36	14.1
3	Pentane	36.074	115.205	25.2656	26.42	196.62	33.31	16.00
4	2-methyl butane	27.852	116.426	25.2923	24.59	187.70	32.9	15.00
5	2,2 dimethyl propane	9.503	112.074	25.7243	21.78	160.60	31.57	12.05
6	Hexane	68.740	130.688	29.9066	31.55	234.70	29.92	18.42
7	2-methyl pentane	60.271	131.933	29.9459	29.86	224.90	29.95	17.38
8	3- methyl pentane	63.282	129.717	29.8016	30.27	231.20	30.83	18.12
9	2,2-dimethyl butane	49.741	132.744	29.9347	27.69	216.20	30.67	16.30
10	2,3- dimethyl butane	57.988	130.240	29.8104	29.12	227.10	30.99	17.37
11	Heptanes	98.427	146.540	34.5504	36.55	267.55	27.01	20.26
12	2-methyl hexane	90.052	147.656	34.5908	34.80	257.90	27.2	19.29
13	3- methyl hexane	91.850	145.821	34.4597	35.08	262.40	28.1	19.79
14	3-ethylpentane	93.475	143.517	34.2827	35.22	267.60	28.6	20.44
15	2,2-dimethyl pentane	79.197	148.695	34.6166	32.43	247.70	28.4	18.02
16	2,3- dimethyl pentane	89.784	144.153	34.3237	34.24	264.60	29.2	19.96
17	2,4- dimethyl pentane	80.500	148.949	34.6192	32.88	247.10	27.4	18.15
18	3,3- dimethyl pentane	86.064	144.530	34.3323	33.02	263.00	30	19.59
19	Octane	125.665	162.592	39.1922	41.48	296.20	24.64	21.76
20	2-methylheptane	117.647	163.663	39.2316	39.68	288.00	24.8	20.60
21	3- methylheptane	118.925	161.832	39.1001	39.83	292.00	25.6	21.17
22	4- methylheptane	117.709	162.105	39.1174	39.67	290.00	25.6	21.00
23	3-ethylhexane	118.53	160.07	38.94	39.40	292.00	25.74	21.51
24	2,2-dimethylhexane	10.84	164.28	39.25	37.29	279.00	25.6	19.60
25	2,3- dimethylhexane	115.607	160.39	38.98	38.79	293.00	26.6	20.99
26	2,4- dimethylhexane	109.42	163.09	39.13	37.76	282.00	25.8	20.05
27	2,5- dimethylhexane	109.10	164.69	39.25	37.86	279.00	25	19.73
28	3,3- dimethylhexane	111.96	160.87	39.00	37.93	290.84	27.2	20.63
29	3,4- dimethylhexane	117.72	158.81	38.84	39.02	298.00	27.4	21.64
30	3-ethyl-2-methylpentane	115.65	158.79	38.83	38.52	295.00	27.4	21.52
31	3-ethyl-3-methylpentane	118.25	157.02	38.71	37.99	305.00	28.9	21.99
32	2,2,3-trimethylpentane	109.84	159.52	38.92	36.91	294.00	28.2	20.67
33	2,2,4- trimethylpentane	99.23	165.08	39.26	35.13	271.15	25.5	18.77
34	2,3,3- trimethylpentane	114.76	157.29	38.76	37.22	303.00	29	21.56
35	2,3,4- trimethylpentane	113.46	158.85	38.86	37.61	295.00	27.6	21.14
36	Nonane	150.79	178.71	43.84	46.44	322.00	22.74	22.92
37	2-methyloctane	143.26	179.77	43.87	44.65	315.00	23.6	21.88
38	3-methyloctane	144.18	177.95	43.72	44.75	318.00	23.7	22.34
39	4-methyloctane	142.48	178.15	43.76	44.75	318.30	23.06	22.34
40	3-ethylheptane	143.00	176.41	43.64	44.81	318.00	23.98	22.81
41	4- ethylheptane	141.20	175.68	43.49	44.81	318.30	23.98	22.81
42	2,2-dimethylheptane	132.69	180.50	43.91	42.28	302.00	22.8	20.80
43	2,3- dimethylheptane	140.50	176.65	43.63	43.79	315.00	23.79	22.34
44	2,4- dimethylheptane	133.50	179.12	43.73	42.87	306.00	22.7	23.30
45	2,5- dimethylheptane	136.00	179.37	43.84	43.87	307.80	22.7	21.30
46	2,6- dimethylheptane	135.21	180.91	43.92	42.82	306.00	23.7	20.83
47	3,3- dimethylheptane	137.00	176.897	43.6870	42.66	314.00	24.19	22.01
48	3,4- dimethylheptane	140.600	175.349	43.5473	43.84	322.70	24.77	22.80
49	3,5- dimethylheptane	136.000	177.386	43.6379	42.98	312.30	23.59	21.77
50	4,4- dimethylheptane	135.200	176.897	43.6022	42.66	317.80	24.18	22.01
51	3-ethyl-2-methylhexane	138.000	175.445	43.6550	43.84	322.70	24.77	22.80
52	4-ethyl-2-methylhexane	133.800	177.386	43.6472	42.98	330.30	25.56	21.77
53	3-ethyl-3-methylhexane	140.600	173.077	43.2680	44.04	327.20	25.66	23.22
54	2,2,4-trimethylhexane	126.540	179.220	43.7638	40.57	301.00	23.39	20.51
55	2,2,5- trimethylhexane	124.084	181.346	43.9356	40.17	296.60	22.41	20.04
56	2,3,3- trimethylhexane	137.680	173.780	43.4347	42.23	326.10	25.56	22.41
57	2,3,4- trimethylhexane	139.000	173.498	43.4917	42.93	324.20	25.46	22.80
58	2,3,5- trimethylhexane	131.340	177.656	43.6474	41.42	309.40	23.49	21.27
59	3,3,4- trimethylhexane	140.460	172.055	43.3407	42.28	330.60	26.45	23.27
60	3,3-diethylpentane	146.168	170.185	43.1134	43.36	342.80	26.94	23.75
61	2,2-dimethyl-3-ethylpentane	133.830	174.537	43.4571	42.02	322.60	25.96	22.38
62	2,3-dimethyl-3-ethylpentane	142.000	170.093	42.9542	42.55	338.60	26.94	23.87
63	2,4-dimethyl-3-ethylpentane	136.730	173.804	43.4037	42.93	324.20	25.46	22.80
64	2,2,3,3-tetramethylpentane	140.274	169.495	43.2147	41.00	334.50	27.04	23.38
65	2,2,3,4- tetramethylpentane	133.016	173.557	43.4359	41.00	319.60	25.66	21.98
66	2,2,4,4- tetramethylpentane	122.284	178.256	43.8747	38.10	301.60	24.58	20.37
67	2,3,3,4- tetramethylpentane	141.551	169.928	43.2016	41.75	334.50	26.85	23.31

Table 3: Correlation of topological indices with physicochemical properties of Alkane isomers.

	$Bp\left(^{0}\right)$	$ct\left(^{0}C\right)$	$cp\,(atm)$	$mv\left(cm^{3}\right)$	$st\left(\frac{dyne}{cm}\right)$	$hv\,(kJ)$	$mr\left(cm^{3}\right)$
AG_1	0.8463	0.8946	-0.8514	0.9186	0.8308	0.8614	0.9467
SK	0.8211	0.8945	-0.7661	0.8736	0.8097	0.8176	0.927
SK_1	0.8112	0.8959	-0.6730	0.8047	0.8290	0.7910	0.8864
SK_2	0.6841	0.7784	-0.5897	0.8047	0.6870	0.6522	0.7987

$$HV = -0.7 + 0.216AG_1(G) \tag{4.7}$$

$$MR = -1.586 + 0.236AG_1(G) \tag{4.8}$$

2. SK Index

$$Bp = 7.116 + 0.074SK(G) \tag{4.9}$$

$$CT = -4.689 + 0.069SK(G) \tag{4.10}$$

$$CP = 38.327 - 0.867SK(G) \tag{4.11}$$

$$MV = -9.553 + 0.155SK(G) \tag{4.12}$$

$$ST = -7.885 + 1.122SK(G) \tag{4.13}$$

$$HV = -3.07 + 0.478SK(G) \tag{4.14}$$

$$MR = -5.664 + 0.538SK(G) \tag{4.15}$$

3. SK_1 Index

$$Bp = 5.565 + 0.087SK_1(G) \tag{4.16}$$

$$CT = -8.611 + 0.083SK_1(G) \tag{4.17}$$

$$CP = 39.199 - 0.905SK_1(G) \tag{4.18}$$

$$MV = -12.542 + 0.172SK_1(G) \tag{4.19}$$

$$ST = -13.031 + 1.365SK_1(G) \tag{4.20}$$

$$HV = -5.945 + 0.549SK_1(G) \tag{4.21}$$

$$MR = -8.648 + 0.611SK_1(G) \tag{4.22}$$

4. SK_2 Index

$$Bp = 15.014 + 0.182SK_2(G) \tag{4.23}$$

$$CT = -16.102 + 0.178SK_2(G) \tag{4.24}$$

$$CP = 87.24 - 1.965SK_2(G) \tag{4.25}$$

$$MV = -12.542 + 0.172SK_2(G) \tag{4.26}$$

$$ST = -22.813 + 2.802SK_2(G) \tag{4.27}$$

$$HV = -8.052 + 1.122SK_2(G) \tag{4.28}$$

$$MR = -18.07 + 1.364SK_2(G) \tag{4.29}$$

By inspection of the data in Table 4 to Table 7, it is possible to draw a number of conclusions for the given topological indices like invariants.

The QSPR study of $AG_1(G)$ index reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 4, one can easily verify that $AG_1(G)$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $AG_1(G)$ index with physical properties of alkane isomers lies between -0.8514 to 0.9467.

Further, the correlation coefficient value of $AG_1(G)$ index is very high for the MR of alkane isomers with r =0.9467.Thus the QSPR study reveals that the $AG_1(G)$ index is an useful tool in predicting the

Table 4: Statistical parameters for the linear QSPR model for $AG_1(G)$.

Physical Properties	N	a	b	r
Boiling point	67	3.992	0.033	0.8463
Critical temperature	67	-0.976	0.03	0.8946
Critical pressure	67	18.622	-0.414	-0.8514
Molar volume	65	-3.525	0.069	0.9186
ST	67	-2.608	0.495	0.8308
HV	67	-0.7	0.216	0.8614
MR	67	-1.586	0.236	0.9467

Table 5: Statistical parameters for the linear QSPR model for $SK(G)$.

Physical Properties	N	a	b	r
Boiling point	67	7.116	0.074	0.8211
Critical temperature	67	-4.689	0.069	0.8945
Critical pressure	67	38.327	-0.867	-0.7661
Molar volume	65	-9.553	0.155	0.8736
ST	67	-7.885	1.122	0.8097
HV	67	-3.07	0.478	0.8176
MR	67	-5.664	0.538	0.927

Table 6: Statistical parameters for the linear QSPR model for $SK_1(G)$.

Physical Properties	N	a	b	r
Boiling point	67	5.565	0.087	0.8112
Critical temperature	67	-8.611	0.083	0.8959
Critical pressure	67	39.199	-0.905	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-13.031	1.365	0.829
HV	67	-5.945	0.549	0.791
MR	67	-8.648	0.611	0.8864

Table 7: Statistical parameters for the linear QSPR model for $SK_2(G)$.

Physical Properties	N	a	b	r
Boiling point	67	15.014	0.182	0.6841
Critical temperature	67	-16.102	0.178	0.7784
Critical pressure	67	87.24	-1.965	-0.673
Molar volume	65	-12.542	0.172	0.8047
ST	67	-22.813	2.802	0.687
HV	67	-8.052	1.122	0.6522
MR	67	-18.07	1.364	0.7987

physical properties of alkane isomers. The QSPR study of $SK(G)\,index$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 5, one can easily verify that $SK(G)\,index$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK(G)\,\mathtt{index}$ with physical properties of alkane isomers lies between -0.7661 to 0.927. Further, the correlation coefficient value of $SK(G)\,\mathtt{index}$ index is very high for the MR of alkane isomers with r =0.927.Thus the QSPR study reveals that the $SK(G)\,\mathtt{index}$ index is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of $SK_1(G)\,\mathtt{index}$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 6, one can easily verify that $SK_1(G)\,\mathtt{index}$ shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK_1(G)\,\mathtt{index}$ with physical properties of alkane isomers lies between -0.673 to 0.8959. Further, the correlation coefficient value of $SK_1\mathtt{index}$ is very high for the CT of alkane isomers with r =0.8959.Thus the QSPR study reveals that the $SK_1(G)\,\mathtt{index}$ is an useful tool in predicting the physical properties of alkane isomers.

The QSPR study of $SK_2(G)\,\mathtt{index}$ reveals that can be useful in predicting the boiling point, critical temperature, critical pressure, Molar volume, Surface tension, Heat of Vaporisation, Molar refraction of alkane isomers also from Table 7, one can easily verify that $SK_2(G)\,\mathtt{index}$ index shows good correlation with all physical properties of alkane isomers. We can see that the correlation coefficient value of $SK_2(G)\,\mathtt{index}$ with physical properties of alkane isomers lies between -0.673 to 0.7987. Further, the correlation coefficient value of $SK_2(G)\,\mathtt{index}$ is very high for the MR of alkane isomers with r =0.7987.Thus the QSPR study reveals that the $SK_2(G)\,\mathtt{index}$ is an useful tool in predicting the physical properties of alkane isomers.

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Research Article

IJCRR
Section: General Science
Sci. Journal Impact Factor 4.016
ICV: 71.54

Toxicity Effect of Copper on Aquatic Macrophyte (*Pistia Stratiotes* L.)

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ABSTRACT

Industrial development coupled with population growth had resulted in the over exploitation of natural resources. Life support systems viz, water, air and soil are thus getting exposed to an array of pollutants, especially heavy metals released by anthropogenic activities. But tolerant species of aquatic plants are able to survive and withstand the pollution stress and serves as a pollution indicators and as tools for p1hytoremediation of heavy metals from the aquatic ecosystems. Phytoremediation is an biogeotechnological application based on "Green liver concept" and operates on biogeochemical cycling. The present study focuses on copper toxicity on morphology, biochemical parameters and bioaccumulation potential of *Pistia.* The laboratory experiments were conducted for the assay of morphological index parameter (MIP), biochemical parameters and accumulation profile of copper in the test plants at various concentrations viz, 2, 5,10, 15 and 20 ppm, at 4 days regular intervals for 12 days exposure. The test plants show visible symptoms like withering of roots, chlorosis, necrosis and lower leaves gets decayed at higher concentrations (severe at 20 ppm), however, the test plant showed normal growth at lower concentration viz, 2 and 5 ppm. The estimation of biochemical parameters viz, total chlorophyll, protein and carbohydrates of test plants showed significant increase at lower concentrations (2 and 5 ppm) of Cu. The biochemical constituents decreased with increase in exposure concentrations (10, 15 and 20 ppm) and duration. The toxic effect of sewage was directly proportional to its concentrations and exposure duration. The accumulation profile of Cu by Pistia was maximum at 4 days exposure and gradually decreases at subsequent exposure duration.

Key Words: Copper, Accumulation, Toxicity symptoms, Biochemical parameters

INTRODUCTION

Industrialization and urbanization coupled with alarming rate of population growth have resulted in the large scale pollution of aquatic ecosystems by industrial and domestic waste water discharge. Natural erosion and anthropogenic activities are greatly responsible for water pollution particularly heavy metals like Zinc (Zn), Lead (Pb), Cadmium (Cd), Copper (Cu) etc. There is likelihood of phytotoxicity both micro and macrophytes and environmental risks (de-Fillipes and Pallghy, 1994; Wei, et al., 2003). Heavy metals persisting in sediments may be slowly released into the water and become available to the organisms. Some heavy metals viz, Zn, Cu, Iron (Fe), Manganese (Mn) etc. are represented as micronutrients (Reeves and Baker, 2000) and are only toxic when taken in excess quantities (Blaylock and Huang, 2000; Campenela, 2001), but nonessential ions like Pb, Cd and Ni can inhibit various metabolic activities even in small quantities (Cerventes, *et al.,* 2001; Dinkar, *et al.,* 2001; Choudhary and Sharma, 2009).

The waste water emitting from source metals which could be toxic to flora and fauna. Biological treatment of waste water through aquatic macrophytes plants has great potential for its purification, which effectively accumulates the heavy metals (Brix and Schirup, 1989). Aquatic macrophytes accumulate considerable amount of toxic metals and make the environment free from the pollutants. Thus they play significant role in cleaning up of environment and make the environment free from toxic pollutants. So many aquatic plants have been successfully utilized for removing toxic metals from the aquatic environments (Satyakala and Kaiser Jamil 1992). The metal tolerance of plants may be attributed to different enzymes, stress proteins and Phytochelatins (Van-Asche and Clijsters 1990). Accumulation of metals at higher concentra-

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ISSN: 2231-2196 (Print) **ISSN:** 0975-5241 (Online) **DOI:** 10.7324/IJCRR.2017.9153
Received: 03.07.2017 **Revised:** 16.07.2017 **Accepted:** 31.07.2017

tion causes retardation of growth biochemical activities and also generation of –SH group containing enzymes (Weckx and Clijsters 1996).

In the present investigation *Pistia stratiotes*, a common aquatic macrophyte is used to study the effect of different concentrations of copper on morphology, biochemical constituents and accumulation profile of Cu from the experimental pond under laboratory conditions.

MATERIALS AND METHODS

Pistia stratiotes, a free floating aquatic plant from unpolluted water bodies is maintained in cement pots (1 m diameter) under natural conditions at a temperature 28-30^{0}C. About 20 g of young healthy *Pistia* is acclimatized for two weeks in Arnon and Hoagland nutrient solution maintaining pH between 7.1-7.4. The concentrations of Cu in the polluted water are in the range of 02, 05, 10, 15 and 20 mg/l and tap water as a control. Morphological Index parameters (MIP) viz, root length, leaf length and breadth were observed for 12 days at interval of 4 days. Photographs of *Pistia* treated with different concentrations of copper were taken by using Canon's Power Shot G_2 digital camera. For the further study the plants were harvested at the end of 4, 8 and 12 days exposure and are thoroughly washed with distilled water and used for the estimation of total chlorophyll, protein and carbohydrate and also for morphological observations. Plants harvested after 48 hrs were dried at 80^{0}C for 2 days for metal extraction.

The fresh plant sample of 1g is macerated in 100 ml of 80% (v/v) chilled acetone by using pestle and mortar. The centrifuged and supernatant was used for the estimation of total chlorophyll by standard method (Arnon, 1949) using 652 nm against the solvent (80% acetone as a blank). The protein was estimated by Lowry's method (Lowry *et al*., 1951) using Bovine Serum Albumin (BSA) as a standard, using 660 nm and carbohydrates by phenol sulphuric acid method (Dubois *et al*., 1956) using glucose as standard at 490 nm. Morphological characters were identified with the help of photographs, using Canon's Power Shot G_2-digital camera.

The estimation of metal Cu in the test plant was carried out by using standard method (Allen *et al*., 1974). The dried and powdered 1 g plant material was digested by using mixed acid digestion method in Gerhardt digestion unit. The digested samples were diluted with double distilled water and filtered through Whatman filter paper No-44. The estimation of Cu was done by AAS (GBC 932 Plus Austrelia) with air acetylene oxidizing flame and metal hollow cathode lamp at 217.00 nm wavelength. Working standards (SISCOP-Chem-Bombay Lab) were used for the calibration of instrument.

Statistical analysis: Data are presented as mean values ± SE from two independent experiments with three replicates each. Data were subjected to Two - way ANOVA to know significance between concentrations and between exposure duration for the accumulation of heavy metal (Cu). Further, Dunet's test is also applied for multiple comparisons between control and other concentrations. Two – way ANOVA test is also extended to know the significance between concentration and duration for biochemical parameters.

RESULTS

The experiments were conducted with the following parameters:

a. Effect of Copper toxicity on morphology:

The test plant showed luxuriant growth and slight increase in the laminal length and breadth at 5 ppm concentration. The 5 ppm Cu found to promote length by 6.900cm (± 0.047) in comparison to control, 5.33cm (± 0.027) and laminal length 2.63 cm (± 0.047) and breadth, 2.33 cm (± 0.027) when compared to control (laminal length, 1.766 cm ± 0.027 and breadth 1.56cm ± 0.027) respectively during 12 days exposure. However, at 20 ppm Cu, severely inhibit the root length by 1.63 cm (± 0.034) in comparison to control 5.33 cm (± 0.027) and laminal length, 0.80 cm (± 0.047) and breadth, 0.63 cm (± 0.108), when compared to control (laminal length, 1.76 cm ± 0.027 and breadth 1.566 cm ± 0.027) respectively during 12 days exposure (Table 1). MCA test also represented maximum deviation at higher concentration compared to control.

b. Effect of Copper toxicity on biochemical parameters:

The chlorophyll content was very sensitive to copper toxicity. The results found that Cu at 5 ppm found to augment chlorophyll synthesis and was directly proportional to concentration and exposure duration. The chlorophyll content increased by 3.81% (0.381 mg/gm), 4.10% (0.406mg/gm) and 4.79% (0.415mg/gm) respectively at 4, 8 and 12 days exposure compared to control pond. However, the higher concentration of copper found to inhibit the chlorophyll synthesis. The inhibition at 20 ppm Cu by 13.35% (0.318mg/gm), 27.7% (0.284mg/gm) and 46.71% (0.211mg/gm) (significant at $p > 0.95$) at 4, 8 and 12 days exposure respectively compared to control. Two-way ANOVA represents biochemical toxicity to the test plant, concentrations were significant at $p > 0.01$ level but duration is not significant (Fig. 1).

The increase in the carbohydrate content of *Pistia* at 5 ppm Cu by 23.06% (32.0 mg/g), 35.71% (38.0 mg/g) and 36.66% (41.0 mg/g) respectively during 4, 8 and 12 days exposure duration. The severity of inhibition of carbohydrate synthesis was noticed at 20.0 ppm by 46.15% (14.0 mg/g), 57.14% (12.0 mg/g) and 68.75% (10.0 mg/g) respectively at 4, 8 and

12 days exposure in comparison to control (fig.).

The protein synthesis at 5 ppm Cu was promotive irrespective exposure duration. However, the protein content decreased at subsequent higher concentration and inhibition was directly proportional to the duration of exposure. The 5 ppm Cu promoted protein synthesis by 8.06% (6.7 mg/g), 18.75% (7.6 mg/g) and 19.11 (8.1 mg/g) respectively at 4, 8 and 12 days exposure duration. The reduction in protein content was observed with progressive increase in Cu concentration. The inhibition of protein content increase viz, 11.36% (3.9 mg/g), 32.60% and (3.1 mg/g) and 43.75% (2.7 mg/g) was respectively at 4, 8 and 12 days exposure in comparison to respective control (Fig. 1)

Application of two-way ANOVA, it is found that the biochemical responses of test plant species with respect to concentrations were significant at $p < 0.01$ level. However, exposure duration was not statistically significant (Table 2).

c. Profile of Metal Accumulation

The accumulation data (Fig 2) revealed that 'Cu' accumulation in Pistia was directly proportional to its concentration and exposure duration. The Pistia grown in experimental pond containing 5 ppm accumulate 2812.04 µg/g, 3062.0 µg/g and 3208 µg/g and accumulation at higher concentration (20 ppm) was 8425.0µg/g, 8750.0 µg/g and 8770.0 µg/g during 4, 8 and 12 days exposure respectively. Two-way ANOVA showed that both concentration and exposure duration were significant at $p < 0.01$ level in test plants and further Dunet's test was applied for the multiple comparison between control and different concentration treatments of test plant. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table 3).

DISCUSSION

a. Effect of Copper toxicity on morphology: Morphometric assay, is one of the quantitative tool for the assessment of toxicants, was measured by using Morphological Index Parameters (MIP). The rate of inhibition of growth in the root and leaf was directly proportional to the concentrations of copper. The test plant show luxurieant growth and slight increase in the laminal length and breadth at 5 ppm concentration. However, at higher concentration (20 ppm) severely inhibit the root length, laminal length and breadth. Similar observations were made by Garg *et al.*(1994) in *Limnathemum cristastum* at 1 ppm concentration of Pb, Zn and Cr. Our results of toxicity symptoms of copper at higher concentrations observed were similar to Dagon and Saygideger (2011) and Kopitte *et al.,* (2007) and also of Yongpisamshap *et al.,* (2005) in *Salvinia natanas*. Two – way ANOVA states that the concentrations were significantly toxic at 5% level but duration was not significant. MCA test also represented maximum deviation at higher concentration compared to control (Table. 1).

b. Effect of Copper toxicity on biochemical parameters: Copper is essential trace element required by all plants. The accumulation of copper in plants lead to biochemical changes. Total chlorophyll content, a parameter, was a sensitive to heavy metal toxicity (Gupta and Chandra, 1996). Similar observations had been reported by Dhir and Srivastava (2013) in *Salvinia natanas* at 10 ppm of Cu, Fe, Zn, Co and Cr. The stimulation of chlorophyll synthesis may be due to phytochelatins (PCs) which plays role in detoxification (Rolli, *et al* ., 2010) however, the higher concentration of Cu found to inhibit the chlorophyll synthesis. The inhibition at 20 ppm Cu by 13.35% (0.318mg/gm), 27.7% (0.284mg/gm) and 46.71% (0.211mg/gm) (significant at $p > 0.95$) at 4, 8 and 12 days exposure respectively compared to control. Similar observations was made by Singh *et al* 2011 in *Hydrilla verticillata* at higher concentration of Pb at 20 ppm and Cd at 0.05 ppm. This is due to decline in chlorophyll content in plants exposed to Cu due to: 1) inhibition of important enzymes associated with chlorophyll synthesis, 2) peroxidation of chloroplast membranes resulting from heavy metals induced oxidative stress, 3) formation of metal substituted chlorophyll (Patsikka, *et al.*, 2002). Two-way ANOVA represents biochemical toxicity to the test plant, concentrations were significant at $p > 0.01$ level but duration is not significant. Two way ANOVA represents toxicity was at $p > 0.01$ level significant towards but duration was not significant.

Our investigation revealed that lower concentration of copper (5 ppm) promotes the carbohydrate synthesis. The carbohydrate content was increased at lower concentration of Cu, was due to detoxification free radicals by quenching / utilization by enzymatic superoxide dismutase (SOD), peroxidase (POD), catalases or glutathione reductase (Wang *et al.* 1997). Similarly Choudhary and Ramachandra (2005) observed stimulatory effect of carbohydrate in *Nostoc muscorum* at lower concentration (1.5 ppm) of Cu like other heavy metals. But the severity of inhibition of carbohydrate was noticed (Fig. 1). The heavy metals damaged the photosynthetic apparatus, in particular light harvesting complex II (Krupa, 1988) and photosynthesis I and II (Siedlecka and Krupa, 1996) and Hasan *et al.,* (2009).

The proteins play an important role in energy metabolism. In the test plant, the lower concentration of copper enhances the protein synthesis and is directly proportion to exposure duration. However, the protein content was decreased at subsequent higher concentration and inhibition was directly proportional to the exposure duration. Many studies show that protein content of many aquatic macrophyte was increased by accumulation of Pb at lower toxicity concentration. The stimulation of protein synthesis at lower concentration of

Cu (5 ppm) may be attributed to the synthesis of stress proteins. The phytochelatins (PC) and phytochelatin synthetase bind and regulate the Cu and sequesters the toxicity in the plants and thus showed metal tolerance Mohan and Hosetti, 1997; Steffens, 1997). The reduction in protein content was observed with progressive increase in Cu concentration. The inhibition of protein content increase viz, 11.36% (3.9 mg/g), 32.60% and (3.1 mg/g) and 43.75% (2.7 mg/g) was respectively at 4, 8 and 12 days exposure in comparison to respective control (fig. 1)

The proteins played an important role in energy metabolism. A decrease in protein content could be due to inactivation of protein synthesizing enzymes in the cell. The Cu induced oxidative stress by generating reactive oxygen species (ROS). These disrupted cellular homeostasis, thus, enhanced the production of ROS. These ROS reactions with proteins, lipids, nucleic acids causing membrane damage and enzyme content of macrophyte may be due to above reasons (Garg *et al.,* 1994; Romero *et al.,* 2007). (fig. 1)

Application of two-way ANOVA, it is found that the biochemical responses of test plant species with respect to concentrations were significant at $p < 0.01$ level. However, exposure duration was not statistically significant (Table 2).

c. Profile of Metal Accumulation

Heavy metal pollution of a water is a major environmental concern, is increasing at (Dushenkar *et al.* 1995) alarming rate due to anthropogenic activities and is drawing attention and gaining paramanual importance due to its obvious impact on health through the food chain (Prasad 1997). The aquatic plants are able to accumulate heavy metals from sediment water. In the present investigation aquatic macrophyte viz, *Pistia stratiotes* is used in accumulation. The accumulation data (Fig 2) revealed that 'Cu' accumulation in Pistia was directly proportional to its concentration and exposure duration.

It was observed that the rate of accumulation is maximum at 4 days exposure irrespective of concentrations and exposure duration, however, at remaining durations it is marginal. Similar observations were made by Bendra *et al*., (1990) in *Cladophora glomerata* at the concentration of 0.1M solution of Cd. Initial increase in the accumulation might be due to the availability of increased number of binding sites for the complexation of heavy meals ions leading to the increased complexation of heavy metal ions, leading to the increased absorption, however, slow accumulation may be attributed to binding ions to the plants and establishment of equilibrium status between adsorbate and adsorbent (Rai and Kumar, 1999; Sibihi, *et al*., 2012).

Two-way ANOVA showed that both concentration and exposure duration were significant at $p < 0.01$ level in test plants and further Dunet's test was applied for the multiple comparison between control and different concentration treatments of test plant. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table 3)

CONCLUSION

It is concluded from the findings of the present investigation, it is concluded that morphological, biochemical responses and profile of Cu accumulation by *Pistia stratiotes* are directly proportional to concentration of the media and exposure duration. Regular harvest of the plants at the interval of 4 days help to cleanup aquatic environment.

ACKNOWLEDGEMENT

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi (India), Research and Development centre, Bharthiar University, Coimbatore. Dept. of Botany, Karnatak University Dharwad for providing necessary facilities to carry out research work. Further, the author acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also greatful to authors / editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed.

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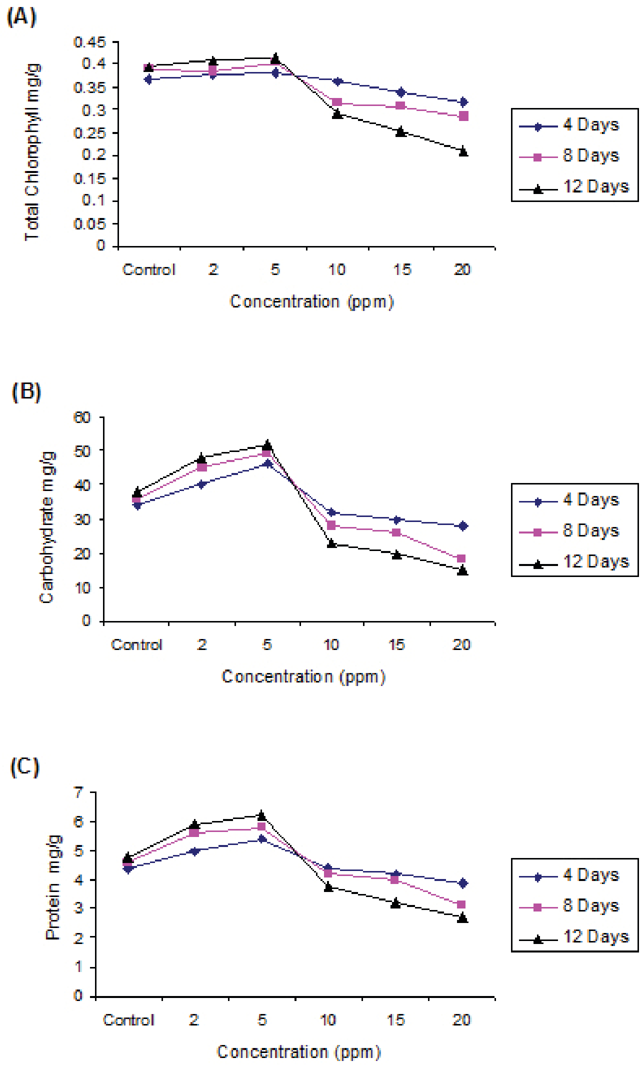

Figure 1: Effect of Copper toxicity on biochemical parameters *(Pistia stratiotes)*
(A) Total Chlorophyll (B) Carbohydrate (C) Protein

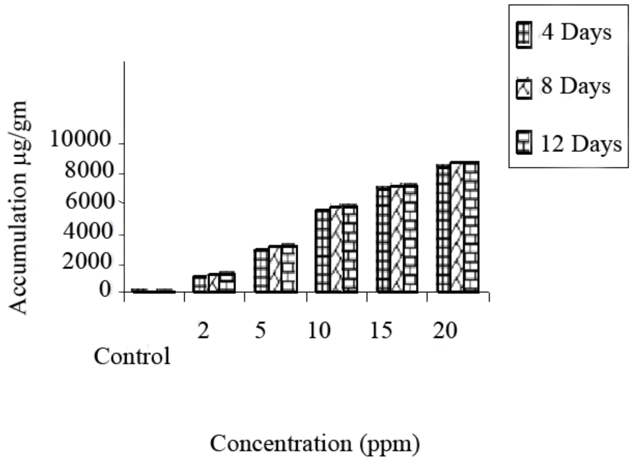

Figure 2: Profile of Metal Accumulation (*Pistia stratiotes)*

Table 1: Effect of Copper toxicity on morphology (*Pistia stratiotes*)

Concentration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	5.266 ± 0.027	5.300 ± 0.124	5.333 ± 0.027	1.700 ± 0.047	1.500 ± 0.047	1.733 ± 0.054	1.500 ± 0.047	1.766 ± 0.027	1.566 ± 0.027
2.0	6.460 ± 0.165	6.566 ± 0.098	6.766 ± 0.098	1.900 ± 0.047	1.600 ± 0.047	1.960 ± 0.054	1.633 ± 0.054	2.000 ± 0.00	1.766 ± 0.027
5.0	7.166 ± 0.072	7.100 ± 0.027	6.900 ± 0.047	2.566 ± 0.054	2.433 ± 0.027	2.600 ± 0.047	2.466 ± 0.047	2.633 ± 0.047	2.333 ± 0.027
10.0	4.933 ± 0.072	4.800 ± 0.047	3.666 ± 0.072	1.466 ± 0.072	1.366 ± 0.072	1.400 ± 0.047	1.266 ± 0.054	1.300 ± 0.047	1.111 ± 0.054
15	3.366 ± 0.118	2.900 ± 0.047	2.700 ± 0.047	1.400 ± 0.047	1.300 ± 0.047	1.333 ± 0.054	1.233 ± 0.072	1.100 ± 0.047	0.900 ± 0.047
20	3.066 ± 0.072	2.766 ± 0.15	1.633 ± 0.0341	1.300 ± 0.047	1.233 ± 0.072	1.133 ± 0.072	0.900 ± 0.094	0.800 ± 0.047	0.63 ± 0.108

Values are expressed in cms

Mean values ± Standard Error

Table 2: Two way ANOVA for biochemical effects of Copper on *Pistia stratiotes*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	7.329**	16.907**	13.090**
F- value (between duration)	1.074	0.363	0.120

** Significant at P < 0.01 level

Table 3: Two way ANOVA with Dunet's test for multiple comparison for accumulation of Copper by *Pistia stratiotes*

	Pistia
F-Value (between concentration)	4687.60
F- value (between duration)	16.59**
Dunet's Value	136.34
Control V/s 2 ppm	1078.66
Control V/s 5ppm	2860.33
Control V/s 10 ppm	5530.33
Control V/s 15 ppm	7016.33
Control V/s 20 ppm	8481.33

** Significant at P < 0.01 level

Research Article

IJCRR
Section: General Science
Sci. Journal Impact Factor 4.016
ICV: 71.54

Toxicity Effect of Copper on Aquatic Macrophyte (*Pistia Stratiotes* L.)

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ABSTRACT

Industrial development coupled with population growth had resulted in the over exploitation of natural resources. Life support systems viz, water, air and soil are thus getting exposed to an array of pollutants, especially heavy metals released by anthropogenic activities. But tolerant species of aquatic plants are able to survive and withstand the pollution stress and serves as a pollution indicators and as tools for p1hytoremediation of heavy metals from the aquatic ecosystems. Phytoremediation is an biogeotechnological application based on "Green liver concept" and operates on biogeochemical cycling. The present study focuses on copper toxicity on morphology, biochemical parameters and bioaccumulation potential of *Pistia.* The laboratory experiments were conducted for the assay of morphological index parameter (MIP), biochemical parameters and accumulation profile of copper in the test plants at various concentrations viz, 2, 5,10, 15 and 20 ppm, at 4 days regular intervals for 12 days exposure. The test plants show visible symptoms like withering of roots, chlorosis, necrosis and lower leaves gets decayed at higher concentrations (severe at 20 ppm), however, the test plant showed normal growth at lower concentration viz, 2 and 5 ppm. The estimation of biochemical parameters viz, total chlorophyll, protein and carbohydrates of test plants showed significant increase at lower concentrations (2 and 5 ppm) of Cu. The biochemical constituents decreased with increase in exposure concentrations (10, 15 and 20 ppm) and duration. The toxic effect of sewage was directly proportional to its concentrations and exposure duration. The accumulation profile of Cu by Pistia was maximum at 4 days exposure and gradually decreases at subsequent exposure duration.

Key Words: Copper, Accumulation, Toxicity symptoms, Biochemical parameters

INTRODUCTION

Industrialization and urbanization coupled with alarming rate of population growth have resulted in the large scale pollution of aquatic ecosystems by industrial and domestic waste water discharge. Natural erosion and anthropogenic activities are greatly responsible for water pollution particularly heavy metals like Zinc (Zn), Lead (Pb), Cadmium (Cd), Copper (Cu) etc. There is likelihood of phytotoxicity both micro and macrophytes and environmental risks (de-Fillipes and Pallghy, 1994; Wei, et al., 2003). Heavy metals persisting in sediments may be slowly released into the water and become available to the organisms. Some heavy metals viz, Zn, Cu, Iron (Fe), Manganese (Mn) etc. are represented as micronutrients (Reeves and Baker, 2000) and are only toxic when taken in excess quantities (Blaylock and Huang, 2000; Campenela, 2001), but nonessential ions like Pb, Cd and Ni can inhibit various metabolic activities even in small quantities (Cerventes, *et al.,* 2001; Dinkar, *et al.,* 2001; Choudhary and Sharma, 2009).

The waste water emitting from source metals which could be toxic to flora and fauna. Biological treatment of waste water through aquatic macrophytes plants has great potential for its purification, which effectively accumulates the heavy metals (Brix and Schirup, 1989). Aquatic macrophytes accumulate considerable amount of toxic metals and make the environment free from the pollutants. Thus they play significant role in cleaning up of environment and make the environment free from toxic pollutants. So many aquatic plants have been successfully utilized for removing toxic metals from the aquatic environments (Satyakala and Kaiser Jamil 1992). The metal tolerance of plants may be attributed to different enzymes, stress proteins and Phytochelatins (Van-Asche and Clijsters 1990). Accumulation of metals at higher concentra-

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ISSN: 2231-2196 (Print)   **ISSN:** 0975-5241 (Online)   **DOI:** 10.7324/IJCRR.2017.9153

Received: 03.07.2017   **Revised:** 16.07.2017   **Accepted:** 31.07.2017

tion causes retardation of growth biochemical activities and also generation of –SH group containing enzymes (Weckx and Clijsters 1996).

In the present investigation *Pistia stratiotes*, a common aquatic macrophyte is used to study the effect of different concentrations of copper on morphology, biochemical constituents and accumulation profile of Cu from the experimental pond under laboratory conditions.

MATERIALS AND METHODS

Pistia stratiotes, a free floating aquatic plant from unpolluted water bodies is maintained in cement pots (1 m diameter) under natural conditions at a temperature 28-30^{0}C. About 20 g of young healthy *Pistia* is acclimatized for two weeks in Arnon and Hoagland nutrient solution maintaining pH between 7.1-7.4. The concentrations of Cu in the polluted water are in the range of 02, 05, 10, 15 and 20 mg/l and tap water as a control. Morphological Index parameters (MIP) viz, root length, leaf length and breadth were observed for 12 days at interval of 4 days. Photographs of *Pistia* treated with different concentrations of copper were taken by using Canon's Power Shot G$_2$ digital camera. For the further study the plants were harvested at the end of 4, 8 and 12 days exposure and are thoroughly washed with distilled water and used for the estimation of total chlorophyll, protein and carbohydrate and also for morphological observations. Plants harvested after 48 hrs were dried at 80^{0}C for 2 days for metal extraction.

The fresh plant sample of 1g is macerated in 100 ml of 80% (v/v) chilled acetone by using pestle and mortar. The centrifuged and supernatant was used for the estimation of total chlorophyll by standard method (Arnon, 1949) using 652 nm against the solvent (80% acetone as a blank). The protein was estimated by Lowry's method (Lowry *et al*., 1951) using Bovine Serum Albumin (BSA) as a standard, using 660 nm and carbohydrates by phenol sulphuric acid method (Dubois *et al*., 1956) using glucose as standard at 490 nm. Morphological characters were identified with the help of photographs, using Canon's Power Shot G$_2$-digital camera.

The estimation of metal Cu in the test plant was carried out by using standard method (Allen *et al*., 1974). The dried and powdered 1 g plant material was digested by using mixed acid digestion method in Gerhardt digestion unit. The digested samples were diluted with double distilled water and filtered through Whatman filter paper No-44. The estimation of Cu was done by AAS (GBC 932 Plus Austrelia) with air acetylene oxidizing flame and metal hollow cathode lamp at 217.00 nm wavelength. Working standards (SISCOP-Chem-Bombay Lab) were used for the calibration of instrument.

Statistical analysis: Data are presented as mean values ± SE from two independent experiments with three replicates each. Data were subjected to Two - way ANOVA to know significance between concentrations and between exposure duration for the accumulation of heavy metal (Cu). Further, Dunet's test is also applied for multiple comparisons between control and other concentrations. Two – way ANOVA test is also extended to know the significance between concentration and duration for biochemical parameters.

RESULTS

The experiments were conducted with the following parameters:

a. Effect of Copper toxicity on morphology:

The test plant showed luxuriant growth and slight increase in the laminal length and breadth at 5 ppm concentration. The 5 ppm Cu found to promote length by 6.900cm (± 0.047) in comparison to control, 5.33cm (± 0.027) and laminal length 2.63 cm (± 0.047) and breadth, 2.33 cm (± 0.027) when compared to control (laminal length, 1.766 cm ± 0.027 and breadth 1.56cm ± 0.027) respectively during 12 days exposure. However, at 20 ppm Cu, severely inhibit the root length by 1.63 cm (± 0.034) in comparison to control 5.33 cm (± 0.027) and laminal length, 0.80 cm (± 0.047) and breadth, 0.63 cm (± 0.108), when compared to control (laminal length, 1.76 cm ± 0.027 and breadth 1.566 cm ± 0.027) respectively during 12 days exposure (Table 1). MCA test also represented maximum deviation at higher concentration compared to control.

b. Effect of Copper toxicity on biochemical parameters:

The chlorophyll content was very sensitive to copper toxicity. The results found that Cu at 5 ppm found to augment chlorophyll synthesis and was directly proportional to concentration and exposure duration. The chlorophyll content increased by 3.81% (0.381 mg/gm), 4.10% (0.406mg/gm) and 4.79% (0.415mg/gm) respectively at 4, 8 and 12 days exposure compared to control pond. However, the higher concentration of copper found to inhibit the chlorophyll synthesis. The inhibition at 20 ppm Cu by 13.35% (0.318mg/gm), 27.7% (0.284mg/gm) and 46.71% (0.211mg/gm) (significant at $p > 0.95$) at 4, 8 and 12 days exposure respectively compared to control. Two-way ANOVA represents biochemical toxicity to the test plant, concentrations were significant at $p > 0.01$ level but duration is not significant (Fig. 1).

The increase in the carbohydrate content of *Pistia* at 5 ppm Cu by 23.06% (32.0 mg/g), 35.71% (38.0 mg/g) and 36.66% (41.0 mg/g) respectively during 4, 8 and 12 days exposure duration. The severity of inhibition of carbohydrate synthesis was noticed at 20.0 ppm by 46.15% (14.0 mg/g), 57.14% (12.0 mg/g) and 68.75% (10.0 mg/g) respectively at 4, 8 and

12 days exposure in comparison to control (fig.).

The protein synthesis at 5 ppm Cu was promotive irrespective exposure duration. However, the protein content decreased at subsequent higher concentration and inhibition was directly proportional to the duration of exposure. The 5 ppm Cu promoted protein synthesis by 8.06% (6.7 mg/g), 18.75% (7.6 mg/g) and 19.11 (8.1 mg/g) respectively at 4, 8 and 12 days exposure duration. The reduction in protein content was observed with progressive increase in Cu concentration. The inhibition of protein content increase viz, 11.36% (3.9 mg/g), 32.60% and (3.1 mg/g) and 43.75% (2.7 mg/g) was respectively at 4, 8 and 12 days exposure in comparison to respective control (Fig. 1)

Application of two-way ANOVA, it is found that the biochemical responses of test plant species with respect to concentrations were significant at $p < 0.01$ level. However, exposure duration was not statistically significant (Table 2).

c. Profile of Metal Accumulation

The accumulation data (Fig 2) revealed that 'Cu' accumulation in Pistia was directly proportional to its concentration and exposure duration. The Pistia grown in experimental pond containing 5 ppm accumulate 2812.04 µg/g, 3062.0 µg/g and 3208 µg/g and accumulation at higher concentration (20 ppm) was 8425.0µg/g, 8750.0 µg/g and 8770.0 µg/g during 4, 8 and 12 days exposure respectively. Two-way ANOVA showed that both concentration and exposure duration were significant at $p < 0.01$ level in test plants and further Dunet's test was applied for the multiple comparison between control and different concentration treatments of test plant. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table 3).

DISCUSSION

a. Effect of Copper toxicity on morphology: Morphometric assay, is one of the quantitative tool for the assessment of toxicants, was measured by using Morphological Index Parameters (MIP). The rate of inhibition of growth in the root and leaf was directly proportional to the concentrations of copper. The test plant show luxurieant growth and slight increase in the laminal length and breadth at 5 ppm concentration. However, at higher concentration (20 ppm) severely inhibit the root length, laminal length and breadth. Similar observations were made by Garg *et al.*(1994) in *Limnathemum cristastum* at 1 ppm concentration of Pb, Zn and Cr. Our results of toxicity symptoms of copper at higher concentrations observed were similar to Dagon and Saygideger (2011) and Kopitte *et al.,* (2007) and also of Yongpisamshap *et al.,* (2005) in *Salvinia natanas*. Two – way ANOVA states that the concentrations were significantly toxic at 5% level but duration was not significant. MCA test also represented maximum deviation at higher concentration compared to control (Table. 1).

b. Effect of Copper toxicity on biochemical parameters: Copper is essential trace element required by all plants. The accumulation of copper in plants lead to biochemical changes. Total chlorophyll content, a parameter, was a sensitive to heavy metal toxicity (Gupta and Chandra, 1996). Similar observations had been reported by Dhir and Srivastava (2013) in *Salvinia natanas* at 10 ppm of Cu, Fe, Zn, Co and Cr. The stimulation of chlorophyll synthesis may be due to phytochelatins (PCs) which plays role in detoxification (Rolli, *et al* ., 2010) however, the higher concentration of Cu found to inhibit the chlorophyll synthesis. The inhibition at 20 ppm Cu by 13.35% (0.318mg/gm), 27.7% (0.284mg/gm) and 46.71% (0.211mg/gm) (significant at $p > 0.95$) at 4, 8 and 12 days exposure respectively compared to control. Similar observations was made by Singh *et al* 2011 in *Hydrilla verticillata* at higher concentration of Pb at 20 ppm and Cd at 0.05 ppm. This is due to decline in chlorophyll content in plants exposed to Cu due to: 1) inhibition of important enzymes associated with chlorophyll synthesis, 2) peroxidation of chloroplast membranes resulting from heavy metals induced oxidative stress, 3) formation of metal substituted chlorophyll (Patsikka, *et al.*, 2002). Two-way ANOVA represents biochemical toxicity to the test plant, concentrations were significant at $p > 0.01$ level but duration is not significant. Two way ANOVA represents toxicity was at $p > 0.01$ level significant towards but duration was not significant.

Our investigation revealed that lower concentration of copper (5 ppm) promotes the carbohydrate synthesis. The carbohydrate content was increased at lower concentration of Cu, was due to detoxification free radicals by quenching / utilization by enzymatic superoxide dismutase (SOD), peroxidase (POD), catalases or glutathione reductase (Wang *et al.* 1997). Similarly Choudhary and Ramachandra (2005) observed stimulatory effect of carbohydrate in *Nostoc muscorum* at lower concentration (1.5 ppm) of Cu like other heavy metals. But the severity of inhibition of carbohydrate was noticed (Fig. 1). The heavy metals damaged the photosynthetic apparatus, in particular light harvesting complex II (Krupa, 1988) and photosynthesis I and II (Siedlecka and Krupa, 1996) and Hasan *et al.,* (2009).

The proteins play an important role in energy metabolism. In the test plant, the lower concentration of copper enhances the protein synthesis and is directly proportion to exposure duration. However, the protein content was decreased at subsequent higher concentration and inhibition was directly proportional to the exposure duration. Many studies show that protein content of many aquatic macrophyte was increased by accumulation of Pb at lower toxicity concentration. The stimulation of protein synthesis at lower concentration of

Cu (5 ppm) may be attributed to the synthesis of stress proteins. The phytochelatins (PC) and phytochelatin synthetase bind and regulate the Cu and sequesters the toxicity in the plants and thus showed metal tolerance Mohan and Hosetti, 1997; Steffens, 1997). The reduction in protein content was observed with progressive increase in Cu concentration. The inhibition of protein content increase viz, 11.36% (3.9 mg/g), 32.60% and (3.1 mg/g) and 43.75% (2.7 mg/g) was respectively at 4, 8 and 12 days exposure in comparison to respective control (fig. 1)

The proteins played an important role in energy metabolism. A decrease in protein content could be due to inactivation of protein synthesizing enzymes in the cell. The Cu induced oxidative stress by generating reactive oxygen species (ROS). These disrupted cellular homeostasis, thus, enhanced the production of ROS. These ROS reactions with proteins, lipids, nucleic acids causing membrane damage and enzyme content of macrophyte may be due to above reasons (Garg *et al.,* 1994; Romero *et al.,* 2007). (fig. 1)

Application of two-way ANOVA, it is found that the biochemical responses of test plant species with respect to concentrations were significant at $p < 0.01$ level. However, exposure duration was not statistically significant (Table 2).

c. Profile of Metal Accumulation

Heavy metal pollution of a water is a major environmental concern, is increasing at (Dushenkar *et al.* 1995) alarming rate due to anthropogenic activities and is drawing attention and gaining paramanual importance due to its obvious impact on health through the food chain (Prasad 1997). The aquatic plants are able to accumulate heavy metals from sediment water. In the present investigation aquatic macrophyte viz, *Pistia stratiotes* is used in accumulation. The accumulation data (Fig 2) revealed that 'Cu' accumulation in Pistia was directly proportional to its concentration and exposure duration.

It was observed that the rate of accumulation is maximum at 4 days exposure irrespective of concentrations and exposure duration, however, at remaining durations it is marginal. Similar observations were made by Bendra *et al*., (1990) in *Cladophora glomerata* at the concentration of 0.1M solution of Cd. Initial increase in the accumulation might be due to the availability of increased number of binding sites for the complexation of heavy meals ions leading to the increased complexation of heavy metal ions, leading to the increased absorption, however, slow accumulation may be attributed to binding ions to the plants and establishment of equilibrium status between adsorbate and adsorbent (Rai and Kumar, 1999; Sibihi, *et al*., 2012).

Two-way ANOVA showed that both concentration and exposure duration were significant at $p < 0.01$ level in test plants and further Dunet's test was applied for the multiple comparison between control and different concentration treatments of test plant. From the statistical analysis it is clear that concentration treatments are significantly differ with control (Table 3)

CONCLUSION

It is concluded from the findings of the present investigation, it is concluded that morphological, biochemical responses and profile of Cu accumulation by *Pistia stratiotes* are directly proportional to concentration of the media and exposure duration. Regular harvest of the plants at the interval of 4 days help to cleanup aquatic environment.

ACKNOWLEDGEMENT

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi (India), Research and Development centre, Bharthiar University, Coimbatore. Dept. of Botany, Karnatak University Dharwad for providing necessary facilities to carry out research work. Further, the author acknowledges the immense help received from the scholars whose articles are cited and included in references of this manuscript. The author is also greatful to authors / editors, publishers of all those articles, journals and books from where the literature for this article has been received and discussed.

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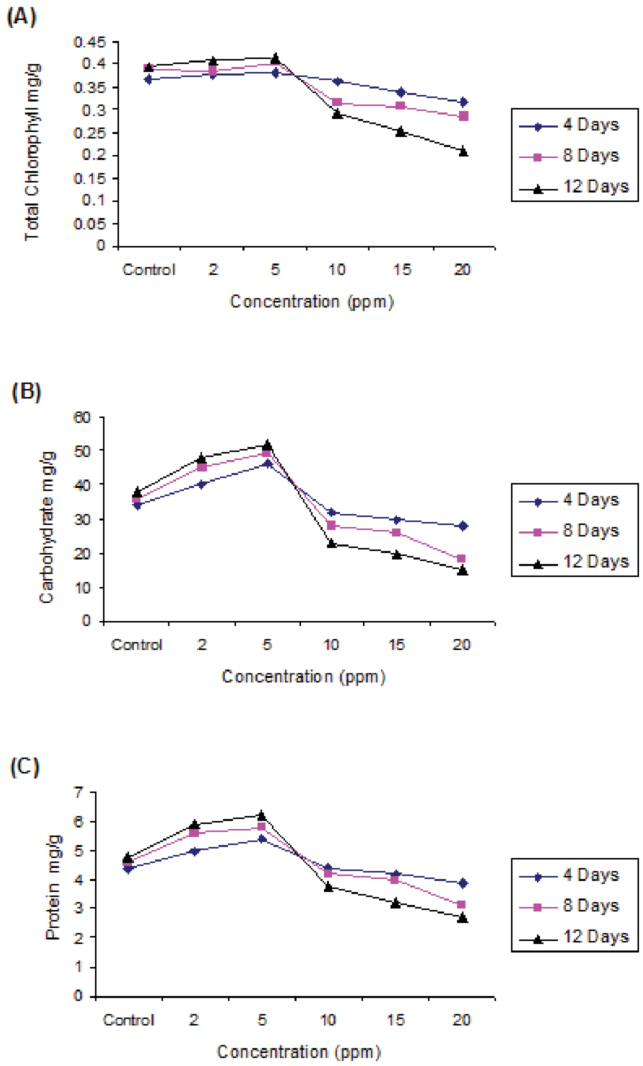

Figure 1: Effect of Copper toxicity on biochemical parameters *(Pistia stratiotes)*
(A) Total Chlorophyll (B) Carbohydrate (C) Protein

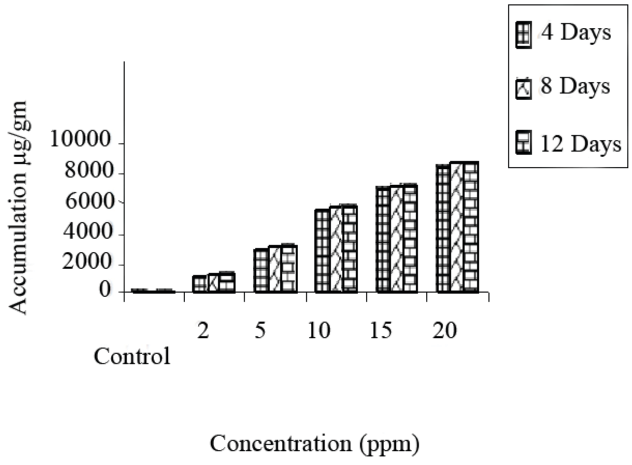

Figure 2: Profile of Metal Accumulation (*Pistia stratiotes)*

Table 1: Effect of Copper toxicity on morphology (*Pistia stratiotes*)

Concen-tration (ppm)	Exposure Duration (in days)								
	4	8	12	4		8		12	
	Root length			Leaf size					
				Length	Breadth	Length	Breadth	Length	Breadth
Control 0	5.266 ± 0.027	5.300 ± 0.124	5.333 ± 0.027	1.700 ± 0.047	1.500 ± 0.047	1.733 ± 0.054	1.500 ± 0.047	1.766 ± 0.027	1.566 ± 0.027
2.0	6.460 ± 0.165	6.566 ± 0.098	6.766 ± 0.098	1.900 ± 0.047	1.600 ± 0.047	1.960 ± 0.054	1.633 ± 0.054	2.000 ± 0.00	1.766 ± 0.027
5.0	7.166 ± 0.072	7.100 ± 0.027	6.900 ± 0.047	2.566 ± 0.054	2.433 ± 0.027	2.600 ± 0.047	2.466 ± 0.047	2.633 ± 0.047	2.333 ± 0.027
10.0	4.933 ± 0.072	4.800 ± 0.047	3.666 ± 0.072	1.466 ± 0.072	1.366 ± 0.072	1.400 ± 0.047	1.266 ± 0.054	1.300 ± 0.047	1.111 ± 0.054
15	3.366 ± 0.118	2.900 ± 0.047	2.700 ± 0.047	1.400 ± 0.047	1.300 ± 0.047	1.333 ± 0.054	1.233 ± 0.072	1.100 ± 0.047	0.900 ± 0.047
20	3.066 ± 0.072	2.766 ± 0.15	1.633 ± 0.0341	1.300 ± 0.047	1.233 ± 0.072	1.133 ± 0.072	0.900 ± 0.094	0.800 ± 0.047	0.63 ± 0.108

Values are expressed in cms

Mean values ± Standard Error

Table 2: Two way ANOVA for biochemical effects of Copper on *Pistia stratiotes*

	Total chlorophyll	Carbohydrate	Protein
F-Value (between concentration)	7.329**	16.907**	13.090**
F- value (between duration)	1.074	0.363	0.120

** Significant at P < 0.01 level

Table 3: Two way ANOVA with Dunet's test for multiple comparison for accumulation of Copper by *Pistia stratiotes*

	Pistia
F-Value (between concentration)	4687.60
F- value (between duration)	16.59**
Dunet's Value	136.34
Control V/s 2 ppm	1078.66
Control V/s 5ppm	2860.33
Control V/s 10 ppm	5530.33
Control V/s 15 ppm	7016.33
Control V/s 20 ppm	8481.33

** Significant at P < 0.01 level

IMPACT FACTOR – 4.23
LangLit
ISSN 2349-5189
An International Peer-Reviewed Open Access Journal
UGC Approved Journal – Arts & Humanities – Sr. No. 49124

DISQUIETS IN GRAHAM SWIFT'S WAR FICTIONS

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ABSTRACT

The central issue discussed in Swift's fiction is concern with war history. In fact this is the common fact of Swift criticism, and even a cursory glance at the novels will show what degree they are fascinated with war and historical events processes for example, dates are extremely prominent in all of Swift's novels; the reader's attention is constantly drawn to the particular year or month of events, as in a historical account. In addition; these dates and characters' experiences are constantly related to Grand National occurrences and developments of Wars. Swift constantly inter-weaves the personal and the historical character lives are deformed and formed by their involvement in the events and processes of their particular time and place in war. Swift's emphasis on war is because wars with their enormous upheavals and savage destruction show the brute force of history in clear terms.

History is replete with unanswered questions regarding our own past and that of the world in which we live. Some of these questions are mere curiosities; others are of the profoundest importance to our cultural identity and have a serious bearing on our future. The central issue discussed in Swift's fiction is concern with war history. In fact this is the common fact of Swift criticism, and even a cursory glance at the novels will show what degree they are fascinated with war and historical events processes for example, dates are extremely prominent in all of Swift's novels; the reader's attention is constantly drawn to the particular year or month of events, as in a historical account. In addition; these dates and characters' experiences are constantly related to Grand National occurrences and developments of Wars.

The term disquiets means anxiety, disturbance, restlessness and impatience and up course all these shadows of war affects the people and also the society in larger scale. And all these were highlighted by Graham Swift in his war based fictions.

War fiction is one of the literary genres in English literature, in which the primary action takes place on battlefield or in home where the characters are either preoccupied with the preparations for war, suffering of or recovering from war.

The war novels origins in the classical and medieval period especially Homer's Iliad Vergil's the Aeneid like old English Beowulf all these epics were concerned with war history or mythology of conflicts between different societies were highlighted war disquiets' and that could reinforce the collective memory of a people.

The war novels developed during the 19th century with works like Stendhal's *The Character House of Parme* (1839) which features the battle of water loo. Leo Tolstoy's *War and Peace* (1869) is depicts the Napoleonic wars in Russia and Stephen Crane's *The Red Budge of Courage*(1895) which deals about the American civil war all these novels features the disquiets and realistic picture of major battles scenes of war time horror and atrocities .

World war- I produced good many number of war novels by the writers from across the world. Some important writers of this time are French writer Henri Barbusse's Le *Feu* (1916) it through light on nationalist dogma and military incompetence. Rebecca West's *The Return of the Soldier* (1918) is about re-integration of shell shocked British soldier into society. John Dos Passos's *Three Soldiers* (1921) Lawrence Stallings autobiographical war novel Plumes published in 1924. Richard Aldington's *Death of a Hero* (1929) Ernest Heming way's *A Farewell to Arms* (1929) all deals with war disquiets.

During 1930's historical novels which deals with earlier war themes were became popular. Margaret Mitchells *Gone with the wind* (1936) which recalls American civil war. William Faulkner's *the unvanquished* (1938) is deals with civil war.

Second World War gave rise to a new boom in contemporary war novels. Unlike world war – I dominated by Europeans world war –II novels were highly produced by American writers they are James Jones's *From Here to Eternity* and Hemingway's *For Whom the Bell Tolls* were deals about Spanish civil war. Jean Paul Sartre *Troubled Sleep* depicts the fall of France in 1940. The bombing incident on London in 1940-41 is the main subject of three British novels published in 1943 are Graham Greene's *The Ministry of Fear* , James Hanley's *No Direction* , Henry Greene's *Caught*, Elizabeth Bowen's *The Heat of the day* (1948) Joseph Heller's Satirical *cat*-22, Norman Mailers *The Naked and the Dead* were deals with war themes. Michael on Datje the *English Patient* is a 1922 booker prize winning novel set in Italian campaign of world war-II.

Immediately after the world war –II we have Korean and Vietnam wars and these issue attracted the good many number of novelists ex- Graham Greene's The Quite American was depicts the origins of Vietnam war of the 1950. Tim O Brien's The Things They Carried is about Vietnam War. Ian MacEwans novels Black dogs and Atonement deals with the issues of world war-II. The post 9/11 event gives terrorism as the most significant subject matter for the literary world to produce few novels ex- Chris Cleave's *Incendiary* (2005) it addresses the event Bombing on London in 2005.

Like all the above mentioned novelists novels were artistically depicts the Horror, wounds and pictures the disquiets of war. Likewise graham Swift's novels were also addresses the issues and events of war. Swift never Claimed that he is a war fiction writer but the issues and events he addresses and discusses in his work of art/ novels themselves made it clear that Graham Swift is also one of the most important war writer of the later 20th century and 21st century.

Graham Swift was brought up in the company of his grandfather, was a war veteran and he use to tell the war based stories to Graham Swift in his childhood days in this sense the seed of war is shallowed in to Graham Swifts mind later he used this element in his writings.

Grand events impinge, too above all in the shape of war. Almost all major character in swift's novels is affected in some way by twentieth century war-fare especially by the Second World War. Willy Chapman is unusual in his detachment from armed conflict, but even he thinks a lot about the war during its course, although it scarcely touches him directly. The heroic fathers in *Shuttlecock* and *Ever-After* are the military veterans whose lives and their son's lives have been affected and shaped by the Second World War. In *Last Orders* Jack Dodd's meets Ray Johnson while serving with the British army in Egypt in 1940s, Lenny Tate's career as a boxer is destroyed by his six years in the army, Vic Tuckers view of the world is partially shaped by his experiences in the Royal Navy. In W*aterland*, many of the events in the fens are set against a backdrop of the war in Europe. Flights of U.S. bombers take off from the Fenland to bomb Hamburg. Tom gains a sense of the importance and fragility of civilization in bombed-out German cities.

Other twentieth century conflicts lives too. Robert Beech in *Out of this World* is badly wounded during the First World War and is killed by bomb, while his son Harry makes his career out of photographing the wars of the later twentieth century. Vince Dodd's in *Lost Orders* learns his trade and some of his attitudes in the British army as it fights to hold on to and then withdraws from Aden in the 1960s. In *The Light of the Day* Christiana is a Croatian refugee from the Balkan wars of the 1990s. Swift constantly inter-weaves the personal and the historical character lives are deformed and formed by their involvement in the events and processes of their particular time and place in war. Swift's emphasis on war is because wars with their enormous upheavals and savage destruction show the brute force of history in clear terms. Robert Beech and Henry Crick are literally the walking wounded of history.

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Hindawi Publishing Corporation
Journal of Mathematics
Volume 2016, Article ID 4341919, 6 pages
http://dx.doi.org/10.1155/2016/4341919

Research Article

Computation of New Degree-Based Topological Indices of Graphene

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Received 24 June 2016; Revised 26 August 2016; Accepted 7 September 2016

Academic Editor: Wai Chee Shiu

Graphene is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Inspired by recent work on Graphene of computing topological indices, here we propose new topological indices, namely, Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, and SK_2 index of a molecular graph G and obtain the explicit formulae of these indices for Graphene.

1. Introduction

A topological index of a chemical compound is an integer, derived following a certain rule, which can be used to characterize the chemical compound and predict certain physiochemical properties like boiling point, molecular weight, density, refractive index, and so forth [1, 2].

A molecular graph $G = (V, E)$ is a simple graph having $n = |V|$ vertices and $m = |E|$ edges. The vertices $v_i \in V$ represent nonhydrogen atoms and the edges $(v_i, v_j) \in E$ represent covalent bonds between the corresponding atoms. In particular, hydrocarbons are formed only by carbon and hydrogen atom and their molecular graphs represent the carbon skeleton of the molecule [1, 2].

Molecular graphs are a special type of chemical graphs, which represent the constitution of molecules. They are also called constitutional graphs. When the constitutional graph of a molecule is represented in a two-dimensional basis, it is called structural graph [1, 2].

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by du and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [3].

2. Computing the Topological Indices of Graphene

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industrialists worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Also it is the most effective material for electromagnetic interference (EMI) shielding. Now we focus on computation of topological indices of Graphene [4–6].

Motivated by previous research on Graphene, here we introduce four new topological indices and computed their corresponding topological index value of Graphene [7–13].

In Figure 1, the molecular graph of Graphene is shown.

2.1. Motivation

2.1. Motivation. By looking at the earlier results for computing the topological indices for Graphene, here we introduce new degree-based topological indices to compute their values for Graphene.

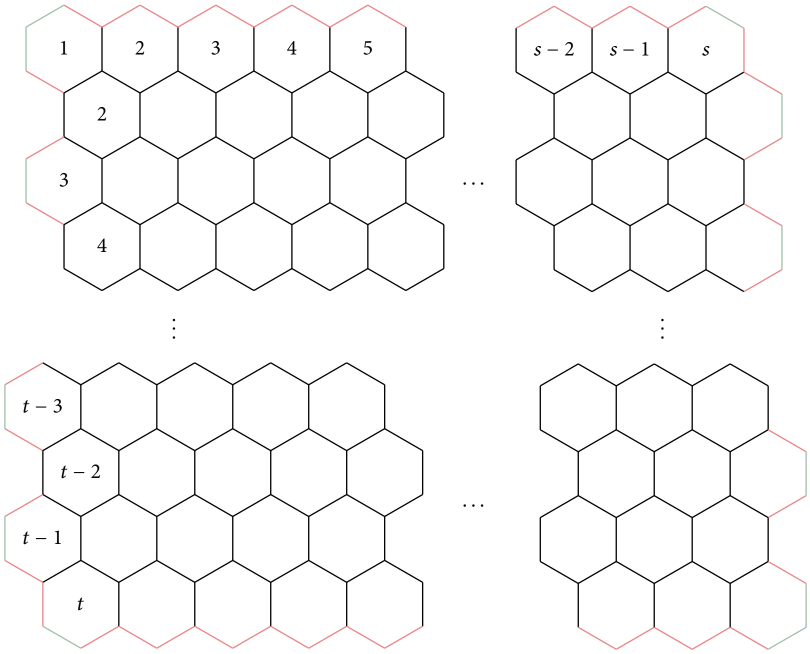

Figure 1

In the upcoming sections, topological indices and their computation of topological indices for Graphene are discussed.

Definition 1 (Arithmetic-Geometric (AG_1) index). Let $G = (V, E)$ be a molecular graph and du be the degree of the vertex u; then AG_1 index of G is defined as

$$AG_1(G) = \sum_{u,v\in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) \cdot d_G(v)}}, \tag{1}$$

where AG_1 index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denote the degree of the vertex u (or v).

Definition 2 (SK index). The SK index of a graph $G = (V, E)$ is defined as $SK(G) = \sum_{u,v\in E(G)}((d_G(u) + d_G(v))/2)$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G, respectively.

Definition 3 (SK_1 index). The SK_1 index of a graph $G = (V, E)$ is defined as $SK_1(G) = \sum_{u,v\in E(G)}((d_G(u) \cdot d_G(v))/2)$, where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G, respectively.

Definition 4 (SK_2 index). The SK_2 index of a graph $G = (V, E)$ is defined as $SK_2(G) = \sum_{u,v\in E(G)}((d_G(u) + d_G(v))/2)^2$, where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G, respectively.

Table 1

Row	$m_{2,2}$	$m_{2,3}$	$m_{3,3}$
1	3	$2s$	$3s - 2$
2	1	2	$3s - 1$
3	1	2	$3s - 1$
4	1	2	$3s - 1$
⋮	⋮	⋮	⋮
t	3	$3s$	$s - 1$
Total	$t + 4$	$4s + 2t - 4$	$3ts - 2s - t - 1$

3. Main Results

Theorem 5. *The AG_1 index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$AG_1(G) = \begin{cases} \dfrac{6\sqrt{6}st + (20 - 4\sqrt{6})s + 10t - (20 - 6\sqrt{6})}{2\sqrt{6}}, & \text{if } t \neq 1 \\ \dfrac{(2\sqrt{6} + 20)s + 6\sqrt{6} - 10}{2\sqrt{6}}, & \text{if } t = 1. \end{cases} \tag{2}$$

Proof. Consider a Graphene having "t" rows with "s" Benzene rings in each row. Let $m_{i,j}$ denote the number of edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of Graphene (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

Therefore Graphene contains $m_{2,2} = (t+4)$ edges, $m_{2,3} = (4s+2t-4)$ edges, and $m_{3,3} = (3ts-2s-t-1)$ edges.

$$\begin{aligned}
\mathrm{AG}_1(G) &= \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)\cdot d_G(v)}},\\
\mathrm{AG}_1(G) &= m_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right) + m_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right)\\
&\quad + m_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right)\\
&= (t+4)\left(\frac{4}{4}\right) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right)\\
&\quad + (3ts-2s-t-1)\left(\frac{6}{6}\right)\\
&= (t+4) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right) + 3ts - 2s\\
&\quad - t - 1\\
&= (3ts-2s+3) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right)\\
&= \frac{2\sqrt{6}(3ts-2s+3) + 5(4s+2t-4)}{2\sqrt{6}}\\
&= \frac{6\sqrt{6}ts - 4\sqrt{6}s + 6\sqrt{6} + 20s + 10t - 20}{2\sqrt{6}}\\
&= \frac{6\sqrt{6} + \left(20-4\sqrt{6}\right)s + 10t - \left(20-6\sqrt{6}\right)}{2\sqrt{6}}.
\end{aligned} \tag{3}$$

Now consider the following cases.

Case 1. The Arithmetic-Geometric index of Graphene for $t \neq 1$ is

$$\mathrm{AG}_1(G) = \frac{6\sqrt{6} + \left(20-4\sqrt{6}\right)s + 10t - \left(20-6\sqrt{6}\right)}{2\sqrt{6}}. \tag{4}$$

Case 2. $t = 1$, $m_{2,2} = t+4$, $m_{2,3} = 4s-2$, and $m_{3,3} = s-2$, edges as shown in Figure 2:

$$\begin{aligned}
\mathrm{AG}_1(G) &= \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u)\cdot d_G(v)}},\\
\mathrm{AG}_1(G) &= m_{2,2}\left(\frac{2+2}{2\sqrt{2.2}}\right) + m_{2,3}\left(\frac{2+3}{2\sqrt{2.3}}\right)\\
&\quad + m_{3,3}\left(\frac{3+3}{2\sqrt{3.3}}\right)\\
&= (t+4)\left(\frac{4}{4}\right) + (4s+2t-4)\left(\frac{5}{2\sqrt{6}}\right)\\
&\quad + (3ts-2s-t-1)\left(\frac{6}{6}\right)\\
&= 5(1) + (4s-2)\left(\frac{5}{2\sqrt{6}}\right) + (s-2)(1)\\
&= s + 3 + (4s-2)\left(\frac{5}{2\sqrt{6}}\right)\\
&= \frac{2\sqrt{6}(s) + 6\sqrt{6} + 20s - 10}{2\sqrt{6}}\\
&= \frac{\left(2\sqrt{6}+20\right)s + 6\sqrt{6} - 10}{2\sqrt{6}}.
\end{aligned} \tag{5}$$

□

Theorem 6. *The SK index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$SK(G) = \begin{cases} \dfrac{18ts + 8s + 8t - 10}{2}, & \textit{if } t \neq 1\\[2mm] \dfrac{26s - 2}{2}, & \textit{if } t = 1. \end{cases} \tag{6}$$

Proof. Consider Graphene having "t" rows with "s" Benzene rings in each row. Let $m_{i,j}$ denote the number of edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of Graphene (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

Therefore, Graphene contains $m_{2,2} = (t+4)$ edges, $m_{2,3} = (4s+2t-4)$ edges, and $m_{3,3} = (3ts-2s-t-1)$ edges.

$$\begin{aligned}
SK(G) &= \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2},\\
SK(G) &\\
&= m_{2,2}\left(\frac{2+2}{2}\right) + m_{2,3}\left(\frac{2+3}{2}\right) + m_{3,3}\left(\frac{3+3}{2}\right)\\
&= (t+4)\left(\frac{4}{2}\right) + (4s+2t-4)\left(\frac{5}{2}\right)\\
&\quad + (3ts-2s-1)\left(\frac{6}{2}\right)\\
&= 2(t+4) + (4s+2t-4)\left(\frac{5}{2}\right)\\
&\quad + 3(3ts-2s-t-1)\\
&= 2t + 8 + (4s+2t-4)\left(\frac{5}{2}\right) + 9ts - 6s - 3t - 3\\
&= \frac{4t + 16 + 20s + 10t - 20 + 18ts - 12s - 6t - 6}{2}\\
&= \frac{18ts + 8s + 8t - 10}{2}.
\end{aligned} \tag{7}$$

Now consider the following cases.

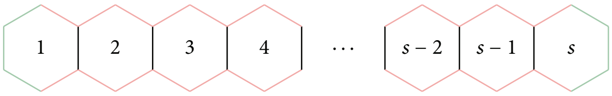

Figure 2

Case 1. The SK index of Graphene for $t \neq 1$ is

$$\mathrm{SK}(G) = \frac{18ts + 8s + 8t - 10}{2}. \tag{8}$$

Case 2. $t = 1$, $m_{2,2} = t + 4$, $m_{2,3} = 4s - 2$, and $m_{3,3} = s - 2$, edges as shown in Figure 2:

$$\begin{aligned} \mathrm{SK}(G) &= \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}, \\ \mathrm{SK}(G) &= m_{2,2}\left(\frac{2+2}{2}\right) + m_{2,3}\left(\frac{2+3}{2}\right) \\ &\quad + m_{3,3}\left(\frac{3+3}{2}\right) \\ &= (t+4)\left(\frac{4}{2}\right) + (4s+2t-4)\left(\frac{5}{2}\right) \\ &\quad + (3ts-2s-t-1)\left(\frac{6}{2}\right). \end{aligned} \tag{9}$$

For $t = 1$,

$$\begin{aligned} &= 5(2) + (4s-2)\left(\frac{5}{2}\right) + (s-2)(3) \\ &= 10 + (4s-2)\left(\frac{5}{2}\right) + 3s - 6 \\ &= \frac{20 + 20s - 10 + 6s - 12}{2} = \frac{26s - 2}{2}. \end{aligned} \tag{10}$$

□

Theorem 7. *The* SK_1 *index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$SK_1(G) = \begin{cases} \dfrac{27ts + 7t + 6s - 17}{2}, & if\ t \neq 1 \\ \dfrac{33s - 10}{2}, & if\ t = 1. \end{cases} \tag{11}$$

Proof. Consider Graphene having "t" rows with "s" Benzene rings in each row. Let $m_{i,j}$ denote the number of edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of Graphene (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

Therefore, Graphene contains $m_{2,2} = (t + 4)$ edges, $m_{2,3} = (4s + 2t - 4)$ edges, and $m_{3,3} = (3ts - 2s - t - 1)$ edges.

$$\begin{aligned} \mathrm{SK}_1(G) &= \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}, \\ \mathrm{SK}_1(G) & \\ &= m_{2,2}\left(\frac{2 \times 2}{2}\right) + m_{2,3}\left(\frac{2 \times 3}{2}\right) + m_{3,3}\left(\frac{3 \times 3}{2}\right) \\ &= (t+4)\left(\frac{4}{2}\right) + (4s+2t-4)\left(\frac{6}{2}\right) \\ &\quad + (3ts-2s-1)\left(\frac{9}{2}\right) \\ &= 2(t+4) + (4s+2t-4)(3) \\ &\quad + (3ts-2s-t-1)\left(\frac{9}{2}\right) \\ &= 2t + 8 + 12s + 6t - 12 + (3ts-2s-t-1)\left(\frac{9}{2}\right) \\ &= \frac{4t + 16 + 24s + 12t - 24 + 27ts - 18s - 9t - 9}{2} \\ &= \frac{27ts + 7t + 6s - 17}{2}. \end{aligned} \tag{12}$$

Now consider the following cases.

Case 1. The SK_1 index of Graphene for $t \neq 1$ is

$$\mathrm{SK}_1(G) = \frac{27ts + 7t + 6s - 17}{2}. \tag{13}$$

Case 2. $t = 1$, $m_{2,2} = t + 4$, $m_{2,3} = 4s - 2$, and $m_{3,3} = s - 2$, edges as shown in Figure 2:

$$\begin{aligned} \mathrm{SK}_1(G) &= \sum_{u,v \in E(G)} \frac{d_G(u) \cdot d_G(v)}{2}, \\ \mathrm{SK}_1(G) &= m_{2,2}\left(\frac{2 \times 2}{2}\right) + m_{2,3}\left(\frac{2 \times 3}{2}\right) \\ &\quad + m_{3,3}\left(\frac{3 \times 3}{2}\right) \\ &= (t+4)\left(\frac{4}{2}\right) + (4s+2t-4)\left(\frac{6}{2}\right) \\ &\quad + (3ts-2s-1)\left(\frac{9}{2}\right) \\ &= 2(t+4) + (4s+2t-4)(3) \\ &\quad + (3ts-2s-t-1)\left(\frac{9}{2}\right). \end{aligned} \tag{14}$$

For $t = 1$,

$$\begin{aligned} &= 2(1+4) + (4s-2)3 + (s-2)\left(\frac{9}{2}\right) \\ &= 10 + 12s - 6 + (s-2)\left(\frac{9}{2}\right) \\ &= \frac{20 + 24s - 12 + 9s - 18}{2} = \frac{33s - 10}{2}. \end{aligned} \tag{15}$$

□

Theorem 8. *The* SK_2 *index of Graphene having "t" rows of Benzene rings with "s" Benzene rings in each row is given by*

$$SK_2(G) = \begin{cases} \dfrac{108ts + 30t + 28s - 72}{4}, & if\ t \neq 1 \\ \dfrac{136s - 42}{4}, & if\ t = 1. \end{cases} \tag{16}$$

Proof. Consider Graphene having "t" rows with "s" Benzene rings in each row. Let $m_{i,j}$ denote the number of edges connecting the vertices of degrees d_i and d_j. Two-dimensional structure of Graphene (Figure 1) contains only $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edges. The number of $m_{2,2}$, $m_{2,3}$, and $m_{3,3}$ edge in each row is mentioned in Table 1.

Therefore, Graphene contains $m_{2,2} = (t+4)$ edges, $m_{2,3} = (4s + 2t - 4)$ edges, and $m_{3,3} = (3ts - 2s - t - 1)$ edges.

$$\begin{aligned}
\mathrm{SK}_2(G) &= \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2, \\
\mathrm{SK}_2(G) & \\
&= m_{2,2}\left(\frac{2+2}{2}\right)^2 + m_{2,3}\left(\frac{2+3}{2}\right)^2 + m_{3,3}\left(\frac{3+3}{2}\right)^2 \\
&= (t+4)\left(\frac{4}{2}\right)^2 + (4s+2t-4)\left(\frac{5}{2}\right)^2 \\
&\quad + (3ts-2s-1)\left(\frac{6}{2}\right)^2 \\
&= 4(t+4) + (4s+2t-4)\left(\frac{25}{4}\right) + 9(3ts-2s-t-1) \\
&= 4t + 16 + (4s+2t-4)\left(\frac{25}{4}\right) + 27ts - 18s - 9t - 9 \\
&= \frac{16t + 64 + 100s + 50t - 100 + 108ts - 72s - 36t - 36}{4} \\
&= \frac{108ts + 30t + 28s - 72}{4}.
\end{aligned} \tag{17}$$

Now consider the following cases.

Case 1. The SK_2 index of Graphene for $t \neq 1$ is

$$\mathrm{SK}_2(G) = \frac{108ts + 30t + 28s - 72}{4}. \tag{18}$$

Case 2. $t = 1$, $m_{2,2} = t + 4$, $m_{2,3} = 4s - 2$, and $m_{3,3} = s - 2$, edges as shown in Figure 2:

$$\begin{aligned}
\mathrm{SK}_2(G) &= \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2, \\
\mathrm{SK}_2(G) &= m_{2,2}\left(\frac{2+2}{2}\right)^2 + m_{2,3}\left(\frac{2+3}{2}\right)^2 \\
&\quad + m_{3,3}\left(\frac{3+3}{2}\right)^2 \\
&= (t+4)\left(\frac{4}{2}\right)^2 + (4s+2t-4)\left(\frac{5}{2}\right)^2 \\
&\quad + (3ts-2s-1)\left(\frac{6}{2}\right)^2 \\
&= 4(t+4) + (4s+2t-4)\left(\frac{25}{4}\right) \\
&\quad + 9(3ts-2s-t-1).
\end{aligned} \tag{19}$$

For $t = 1$,

$$\begin{aligned}
&= 4(1+4) + (4s-2)\left(\frac{25}{4}\right) + 9(s-2) \\
&= 20 + (4s-2)\left(\frac{25}{4}\right) + 9s - 18 \\
&= \frac{80 + 100s - 50 + 36s - 72}{4} = \frac{136s - 42}{4}.
\end{aligned} \tag{20}$$

□

3.1. Conclusion. A generalized formula for Arithmetic-Geometric index (AG_1 index), SK index, SK_1 index, and SK_2 index of Graphene has been obtained without using computer.

Competing Interests

The authors declare that there are no competing interests regarding the publication of this paper.

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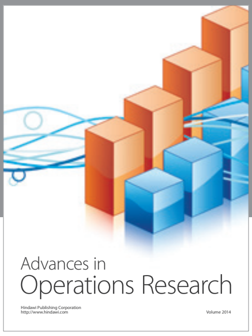
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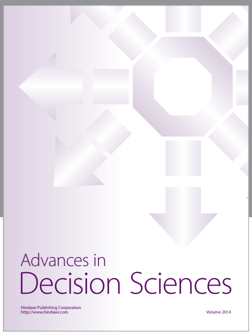
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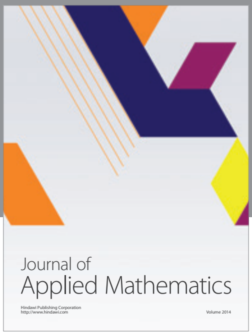
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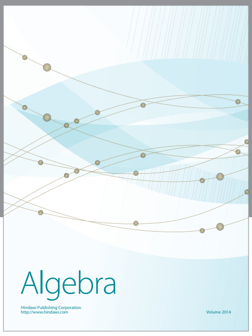
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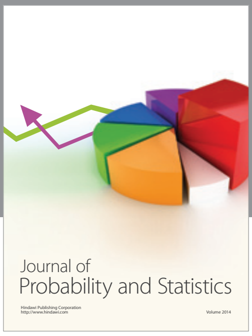
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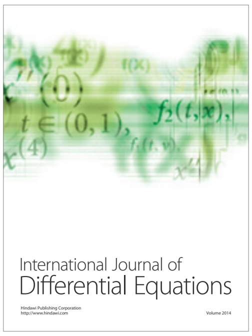
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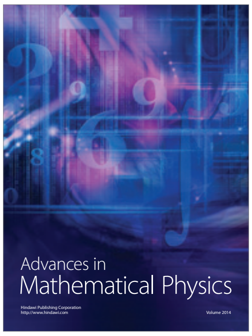
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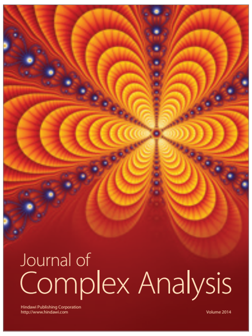
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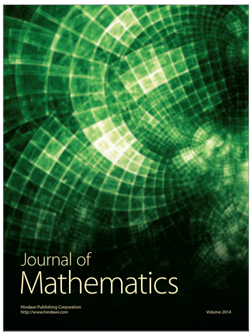
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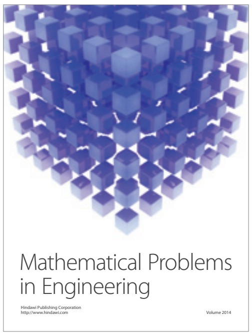
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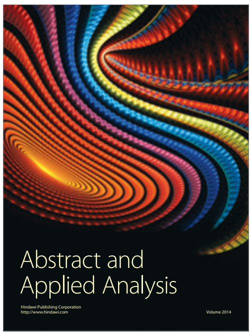
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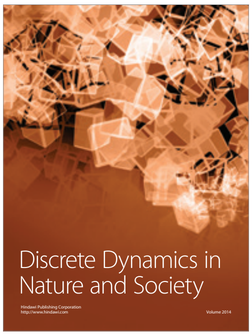
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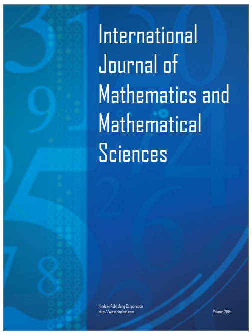
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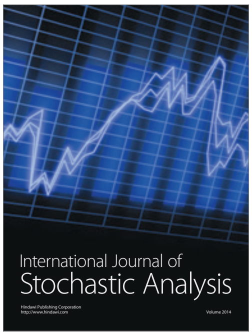
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Shahid Rajaee Teacher Training University

Computing degree-based topological indices of polyhex nanotubes

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Academic Editor: Ali Reza Ashrafi

Abstract. Recently, Shigehalli and Kanabur [17] have put forward for new degree based topological indices, namely geometric-arithmetic index (GA_1 index), SK index, SK_1 index and SK_2 index of a molecular graph G. In this paper, we obtain the explicit formulas of these indices for polyhex nanotube without the aid of a computer.

Keywords. chemical graph, degree-based topological indices, polyhex nanotube.

1 Introduction

A topological index of a chemical compound is an integer, derived following a certain rule, which can be used to characterize the chemical compound and predict certain physio-chemical properties like boiling point, molecular weight, density and refractive index and so forth [2, 19].

A molecular graph $G = (V, E)$ is a simple graph having $n = |V|$ vertices and $m = |E|$ edges. The vertices $v_i \in V$ represent non-hydrogen atoms and the edges $(v_i, v_j) \in E$ represent covalent bonds between the corresponding atoms. In particular, hydrocarbons are formed only by carbon and hydrogen atom and their molecular graphs represent the carbon skeleton of the molecule [2, 19].

Molecular graphs are a special type of chemical graphs, which represent the constitution of molecules. They are also called constitutional graphs. When the constitutional graph of a

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molecule is represented in a two-dimensional basis it is called structural graph [2, 19].

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex $u \in V(G)$ is denoted by $d_u(G)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [6].

2 Computing the topological indices of polyhex nanotube

Motivated by previous research on polyhex nanotube [4, 6, 8–10, 12, 15–17], here we compute the values of four new topological indices of polyhex nanotube.

2.1 Geometric-arithmetic (GA_1) index

Let $G = (V, E)$ be a molecular graph, and d_u is the degree of the vertex u. Then GA_1 index of G is defined as

$$GA_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}},$$

Where GA_1 index is considered for distinct vertices. The above equation is the sum of the ratio of the arithmetic mean and geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

2.2 SK Index

The SK index of a graph $G = (V, E)$ is defined as

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2},$$

where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

2.3 SK_1 Index

The SK_1 index of a graph $G = (V, E)$ is defined as

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}.$$

where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

2.4 SK_2 Index

The SK_2 index of a graph $G = (V, E)$ is defined as

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2} \right)^2,$$

where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

3 Main Results

3.1 Armchair polyhex nanotubes

Consider the armchair polyhex nanotubes $G = TUAC_6[m,n]$, where m denotes number of hexagons in first row and n denotes the number of rows. The number of vertices/atoms of armchair polyhex nanotubes is equal to

$$|V(TUAC_6[m,n])| = 2m(n+2),$$

and the number of edges/bonds is

$$|E(TUAC_6[m,n])| = 3mn + 4m.$$

There are three different kinds of edges of G depending on the degree of terminal vertices of edges.

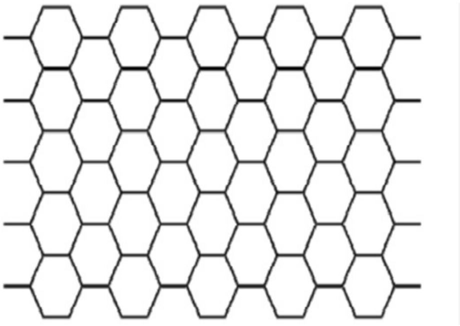

Figure 1. Graph of armchair polyhex $TUAC_6[5,9]$ nanotube.

(d_a, d_b) where $a,b \in E(H)$	(2,2)	(2,3)	(3,3)
Number of edges	2m	4m	3mn − 2m

Table 1. Edge partition of 2D-lattice of H-naphtalenic nanotubes based on degrees of end vertices of each edge.

Theorem 3.1. *Consider the graph of $TUAC_6[m,n]$ nanotubes, then its GA_1 index is equal to*

$$GA_1(TUAC_6[m,n]) = \left(3n + \frac{10}{\sqrt{6}}\right)m.$$

Proof. Consider the $TUAC_6[m,n]$ nanotube. The number of vertices in $TUAC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the geometric-arithmetic index of G which is expressed as

$$GA_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

This implies that

$$\begin{aligned}GA_1(TUAC_6) &= (2,2)\left(\frac{2+2}{2\sqrt{4}}\right) + (2,3)\left(\frac{2+3}{2\sqrt{6}}\right) + (3,3)\left(\frac{3+3}{2\sqrt{9}}\right)\\ &= 2m\,(1) + (4m)\left(\frac{5}{2\sqrt{6}}\right) + (3mn-2m)\,(1)\\ &= 3mn + \frac{10m}{\sqrt{6}}\\ &= \left(3n + \frac{10}{\sqrt{6}}\right)m.\end{aligned}$$

□

Theorem 3.2. *Consider the graph of $TUAC_6[m,n]$ nanotubes, then its SK index is equal to*

$$SK(TUAC_6[m,n]) = (9n+8)\,m.$$

Proof. Consider the $TUAC_6[m,n]$ nanotube. The number of vertices in $TUAC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK index of G which is expressed as

$$SK(G) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2}.$$

This implies that

$$\begin{aligned}SK(TUAC_6[m,n]) &= (2,2)\left(\frac{2+2}{2}\right) + (2,3)\left(\frac{2+3}{2}\right) + (3,3)\left(\frac{3+3}{2}\right)\\ &= 2m\,(2) + 4m\left(\frac{5}{2}\right) + (3mn-2m)\,(3)\\ &= 4m + 10m + 9mn - 6m\\ &= (9n+8)\,m.\end{aligned}$$

□

Theorem 3.3. *Consider the graph of $TUAC_6[m,n]$ nanotubes, then its SK_1 index is equal to*

$$SK_1(TUAC_6[m,n]) = \left(\frac{27n}{2} - 7\right)m.$$

Proof. Consider the $TUAC_6[m,n]$ nanotube. The number of vertices in $TUAC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_1 index of G which is expressed as

$$SK_1(G) = \sum_{u,v\in E(G)} \frac{d_G(u).d_G(v)}{2}.$$

This implies that

$$\begin{aligned}
SK_1(TUAC_6[m,n]) &= (2,2)\left(\frac{2\times 2}{2}\right) + (2,3)\left(\frac{2\times 3}{2}\right) + (3,3)\left(\frac{3\times 3}{2}\right)\\
&= 2m\,(2) + 4m\left(\frac{6}{2}\right) + (3mn-2m)\left(\frac{9}{2}\right)\\
&= 4m + 12m + \frac{27mn}{2} - 9m\\
&= \left(\frac{27n}{2} - 7\right)m.
\end{aligned}$$

□

Theorem 3.4. *Consider the graph of $TUAC_6[m,n]$ nanotubes, then its SK_2 index is equal to*

$$SK_2(TUAC_6[m,n]) = (27n+15)\,m.$$

Proof. Consider the $TUAC_6[m,n]$ nanotube. The number of vertices in $TUAC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_2 index of G which is expressed as

$$SK_2(G) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2.$$

$$\begin{aligned}
SK_2(TUAC_6[m,n]) &= (2,2)\left(\frac{2+2}{2}\right)^2 + (2,3)\left(\frac{2+3}{2}\right)^2 + (3,3)\left(\frac{3+3}{2}\right)^2\\
&= 2m\,(4) + 4m\left(\frac{25}{4}\right) + (3mn-2m)\left(\frac{36}{4}\right)\\
&= 8m + 25m + 27mn - 18m\\
&= (27n+15)\,m.
\end{aligned}$$

□

3.2 Zigzag-edge polyhex nanotubes

Consider the armchair polyhex nanotubes $H = TUZC_6[m,n]$, where m denotes number of hexagons in first row and n denotes the number of rows. The number of vertices/atoms of zigzag-edge polyhex nanotubes is equal to

$$|V(TUZC_6[m,n])| = 2m\,(n+2),$$

and the number of edges/bonds is

$$|E(TUZC_6[m,n])| = 3mn + 4m.$$

There are two different kinds of edges of H depending on the degree of terminal vertices of edges.

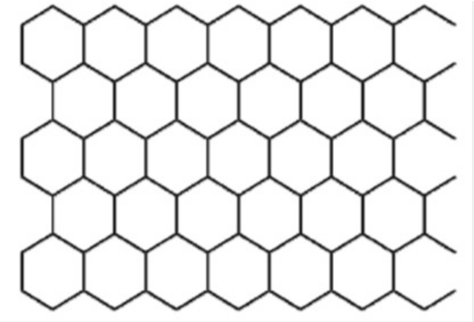

Figure 2. Graph of zigzag edge polyhex TUZC6 [7, 5] nanotube.

(d_a,d_b) where $a,b \in E(H)$	(2,3)	(3,3)
Number of edges	$4m$	$3mn-2m$

Table 2. Edge partition of 2-dimentional graph of $TUZC_6$ nanotube with respect to degree of end vertices of edges.

Theorem 3.5. *Consider the graph of* $TUZC_6[m,n]$ *nanotubes, then its* GA_1 *index is equal to*

$$GA_1(TUAC_6[m,n]) = 3mn + \left(\frac{10}{\sqrt{6}} - 2\right)m.$$

Proof. Consider the $TUZC_6[m,n]$ nanotube. The number of vertices in $TUZC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the geometric-arithmetic index of G which is expressed as

$$GA_1(H) = \sum_{u,v\in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

This implies that

$$\begin{aligned} GA_1(TUZC_6) &= (2,3)\left(\frac{2+3}{2\sqrt{6}}\right) + (3,3)\left(\frac{3+3}{2\sqrt{9}}\right) \\ &= (4m)\left(\frac{5}{2\sqrt{6}}\right) + (3mn-2m)(1) \\ &= \frac{10m}{\sqrt{6}} + 3mn - 2m \\ &= 3mn + \left(\frac{10}{\sqrt{6}} - 2\right)m. \end{aligned}$$

□

Theorem 3.6. *Consider the graph of* $TUZC_6[m,n]$ *nanotubes, then its SK index is equal to*

$$SK(TUZC_6[m,n]) = 9mn + 4m.$$

Proof. Consider the $TUZC_6[m,n]$ nanotube. The number of vertices in $TUZC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK index of G which is expressed as

$$SK(H) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}.$$

This implies that

$$\begin{aligned} SK(TUAC_6[m,n]) &= (2,3)\left(\frac{2+3}{2}\right) + (3,3)\left(\frac{3+3}{2}\right) \\ &= 4m\left(\frac{5}{2}\right) + (3mn-2m)(3) \\ &= 10m + 9mn - 6m \\ &= 9mn + 4m. \end{aligned}$$

□

Theorem 3.7. *Consider the graph of $TUZC_6[m,n]$ nanotubes, then its SK_1 index is equal to*

$$SK_1(TUZC_6[m,n]) = \left(\frac{27n}{2} + 3\right)m.$$

Proof. Consider the $TUZC_6[m,n]$ nanotube. The number of vertices in $TUZC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_1 index of G which is expressed as

$$SK_1(H) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}.$$

This implies that

$$\begin{aligned} SK_1(TUZC_6[m,n]) &= (2,3)\left(\frac{2\times 3}{2}\right) + (3,3)\left(\frac{3\times 3}{2}\right) \\ &= 4m\left(\frac{6}{2}\right) + (3mn-2m)\left(\frac{9}{2}\right) \\ &= 12m + \frac{27mn}{2} - 9m \\ &= \frac{27mn}{2} + 3m \\ &= \left(\frac{27n}{2} + 3\right)m. \end{aligned}$$

□

Theorem 3.8. *Consider the graph of $TUZC_6[m,n]$ nanotubes, then its SK_2 index is equal to*

$$SK_2(TUZC_6[m,n]) = (27n+7)\,m.$$

Proof. Consider the $TUZC_6[m,n]$ nanotube. The number of vertices in $TUZC_6[m,n]$ are $2m(n+2)$ and the number of edges of the nanotube of edges of the nanotube is $3mn+4m$. Now using different type of edges corresponding to the degrees of terminal vertices of edges of G given in Table 1 we compute the SK_2 index of G which is expressed as

$$SK_2(H) = \sum_{u,v\in E(G)} \left(\frac{d_G(u)+d_G(v)}{2}\right)^2.$$

$$\begin{aligned}
SK_2(TUZC_6[m,n]) &= (2,3)\left(\frac{2+3}{2}\right)^2 + (3,3)\left(\frac{3+3}{2}\right)^2\\
&= 4m\left(\frac{25}{4}\right) + (3mn-2m)\left(\frac{36}{4}\right)\\
&= 25m + 27mn - 18m\\
&= 27mn + 7m\\
&= (27n+7)\,m.
\end{aligned}$$

□

Concluding Remarks: A generalized formula for geometric-arithmetic index (GA_1 index), SK index, SK_1 index, SK_2 index for polyhex nanotubes is obtained without using computer.

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New version of degree-based topological indices of certain nanotube

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Academic Editor: Ali Reza Ashrafi

Abstract. In this paper, we compute the geometric-arithmetic index (GA_1 index), SK index, SK_1 index and SK_2 index of H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube. We also compute SK_3 index, GA_2 index for H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube.

Keywords. geometric-arithmetic index (GA_1 index), SK index, SK_1 index, SK_2 index, SK_3 index, GA_2 index, H-naphtalenic nanotube, $TUC_4[m,n]$ nanotube.

1 Introduction

Let G be a simple connected graph in chemical graph theory. In mathematical chemistry, a molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Also a connected graph is a graph such that there is a path between all pairs of vertices. Note that hydrogen atoms are often omitted [6].

Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modelling of chemical phenomena [8, 17, 21, 22]. This theory had an important effect on the development of the chemical sciences.

All molecular graphs considered in this paper are finite, connected, loopless, and without multiple edges. Let $G = (V, E)$ be a graph with n vertices and m edges. The degree of a vertex

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$u \in V(G)$ is denoted by $d_G(u)$ and is the number of vertices that are adjacent to u. The edge connecting the vertices u and v is denoted by uv [9].

2 Computing the topological indices of certain nanotube

Motivated by previous research on certain nanotube, here we introduce six new topological indices and compute their corresponding topological index value of certain nanotube [10, 11, 13, 18–20].

Carbon nanotubes, long, thin cylinders of carbon, were discovered in 1991 by S. Iijima. These are large macromolecules that are unique for their size, shape, and remarkable physical properties. They can be thought of as a sheet of graphite (a hexagonal lattice of carbon) rolled into a cylinder. These intriguing structures have sparked much excitement in recent years and a large amount of research has been dedicated to their understanding. Currently, the physical properties are still being discovered and disputed. Nanotubes have a very broad range of electronic, thermal, and structural properties that change depending on their different kinds (defined by its diameter, length, chirality, or twist). To make things more interesting, besides having a single cylindrical wall (SWNTs), nanotubes can have multiple walls (MWNTs)–cylinders inside other cylinders. Recent work on computing topological indices of certain nanotube can be seen in [10, 11, 14].

The distance between two vertices a and b is denoted as $d_H(a,b)$ and is the length of shortest path between a and b in graph H. The length of shortest path between a and b is also called a-b geodesic. The longest path between any two vertices is called a-b detour.

In this paper, H is considered to be simple connected graph with vertex set $V(H)$ and edge set $E(H)$, da is the degree of vertex $a \in V(H)$ and

$$S_a = \sum_{b \in N_H(a)} d(b),$$

where $N_H = \{b \in V(H) \setminus ab \in E(H)\}$. The notations used in this paper, are mainly taken from books [4, 21]. Now, we propose the following topological indices and compute their value for certain nanotube.

2.1 Geometric-arithmetic- (GA_1) index

Let $G = (V,E)$ be a molecular graph, and d_u be the degree of the vertex u. Then GA_1 index of G is defined as

$$GA_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}},$$

where GA_1 index is considered for distinct vertices. The above equation is the sum of the ratio of the arithmetic mean and geometric mean of u and v, where $d_G(u)$ (or $d_G(v)$) denotes the degree of the vertex u (or v).

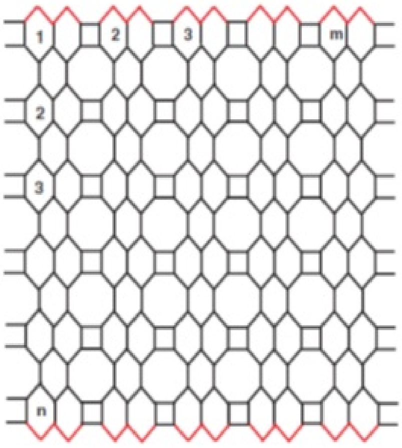

Figure 1. A 2D-lattice of H-naphtalenic nanotube $NPHX[m,n]$ showing the edge partition based on the degrees of end vertices of each edge.

2.2 SK index

The SK index of a graph $G = (V,E)$ is defined as

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2},$$

where $d_G(u)$ and $d_G(v)$ are the degrees of the vertices u and v in G.

2.3 SK_1 index

The SK_1 index of a graph $G = (V,E)$ is defined as

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2},$$

where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

2.4 SK_2 index

The SK_2 index of a graph $G = (V,E)$ is defined as

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2,$$

where $d_G(u)$ and $d_G(v)$ are the product of the degrees of the vertices u and v in G.

2.5 SK_3 index

The SK_3 index of a graph $G = (V,E)$ is defined as

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2},$$

where $S_G(u)$ and $S_G(v)$ are the summation of the degrees of all neighbours of vertices u and v in G.

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

$$N_G(u) = \{v \in V(G) | uv \in E(G)\}.$$

2.6 Geometric-arithmetic (GA_2) index

Let $G = (V, E)$ be a molecular graph, and S_u is the degree of the vertex u, then GA_2 index of G is defined as

$$GA_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}},$$

where GA_2 index is considered for distinct vertices. The above equation is the sum of the ratio of the arithmetic mean and geometric mean of u and v, where $S_G(u)$ (or $S_G(v)$) is the summation of degrees of all neighbours of vertex u (or v).

$$S_G(u) = \sum_{u,v \in E(G)} d_G(u),$$

$$N_G(u) = \{v \in V(G) / uv \in E(G)\}.$$

In this paper, we study certain degree based topological indices of H-naphtalenic nanotubes and $TUC_4[m,n]$ nanotube. These topological indices correlate certain physico-chemical properties of these nanotubes.

3 Main Results

In this paper, we study GA_1, SK, SK_1, SK_2, SK_3 and GA_2 indices of H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube.

3.1 Results for H-naphtalenic nanotubes

In this section, we compute the certain topological indices for H-naphtalenic nanotubes. This nanotube is a trivalent decoration having sequence of C_6, C_6, C_4, C_6, C_6, C_4, ... in first row and a sequence of C_6, C_8, C_6, C_8, ... in other rows. In other words, the whole lattice is a plane tiling that can either cover a cylinder or a torus. These nanotubes are usually symbolized as $NPHX[m,n]$, in which m is the number of pair of hexagons in first row and n is the number of alternative hexagons in a column as depicted in Figure 1. Now we compute certain degree based topological indices for this class of nanotubes. We can clearly see that there are two type of edges in 2D-lattice of this nanotube, as shown by different colours in Figure 1, the colour red shows the edges ab and $d_a = 2$ and $d_b = 3$ and the colour black shows the edges ab with $d_a = d_b = 3$. Table 1 shows cardinalities of these two partite series of edge set of $NPHX[m,n]$ nanotube.

(d_a, d_b) where $a,b \in E(H)$	(2,3)	(3,3)
Number of edges	8m	15mn − 10m

Table 1. Edge partition of 2D-lattice of H-naphtalenic nanotubes based on degrees of end vertices of each edge.

Theorem 3.1. *Consider the graph of $NPHX[m,n]$ nanotubes, then its GA_1 index is equal to*

$$GA_1(NPHX[m,n]) = (15n + 20 - 10\sqrt{6})m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the GA_1 index of $NPHX[m,n]$ nanotube.

$$GA_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

$$\begin{aligned} GA_1(NPHX(n)) &= 8m\left(\frac{2+3}{2\sqrt{6}}\right) + (15mn - 10m)\left(\frac{3+3}{2\sqrt{9}}\right) \\ &= \frac{20m}{\sqrt{6}} + 15mn - 10m \\ &= 15mn + \left(\frac{20}{\sqrt{6}} - 10\right)m \\ &= \left(15n + 20 - 10\sqrt{6}\right)m. \end{aligned}$$

□

Theorem 3.2. *Consider the graph of $NPHX[m,n]$ nanotubes, then its SK index is equal to*

$$SK(NPHX[m,n]) = (45n - 10)m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the SK index of $NPHX[m,n]$ nanotube.

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}.$$

$$\begin{aligned} SK(NPHX(n)) &= 8m\left(\frac{2+3}{2}\right) + (15mn - 10m)\left(\frac{3+3}{2}\right) \\ &= 20m + 45mn - 30m \\ &= 45mn - 10m \\ &= (45n - 10)\,m. \end{aligned}$$

□

Theorem 3.3. *Consider the graph of $NPHX[m,n]$ nanotubes, then its SK_1 index is equal to*

$$SK_1(NPHX[m,n]) = \frac{1}{2}(135n - 42)\,m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the SK_1 index of $NPHX[m,n]$ nanotube.

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}.$$

$$\begin{aligned} SK_1(NPHX(n)) &= 8m\left(\frac{2\times 3}{2}\right) + (15mn - 10m)\left(\frac{3\times 3}{2}\right) \\ &= 24m + (15mn - 10m)\frac{9}{2} \\ &= \frac{1}{2}(48m + 135mn - 90m) \\ &= \frac{1}{2}(135n - 42)\,m. \end{aligned}$$

□

Theorem 3.4. *Consider the graph of $NPHX[m,n]$ nanotubes, then its SK_2 index is equal to*

$$SK_2(NPHX[m,n]) = (135n - 40)\,m.$$

Proof. Consider the graph of $NPHX[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $NPHX[m,n]$ nanotube given in Table 1, we compute the SK_2 index of $NPHX[m,n]$ nanotube.

$$SK_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_G(u) + d_G(v)}{2}\right)^2.$$

$$\begin{aligned} SK_2(NPHX(n)) &= 8m\left(\frac{2+3}{2}\right)^2 + (15mn - 10m)\left(\frac{3+3}{2}\right)^2 \\ &= 50m + 135mn - 90m \\ &= (135n - 40)\,m. \end{aligned}$$

Now we compute two important topological indices GA_2 and SK_3 for 2D-lattice of $NHPX[m,n]$ nanotube. There are six types of edges in $NHPX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge as depicted in Figure 2, in which different colours shows different partite sets of edge set of $NHPX[m,n]$

(S_a, S_b) where $u,v \in E(H)$	(6,7)	(6,8)	(8,8)	(7,9)	(8,9)	(9,9)
Number of edges	$4m$	$4m$	$2m$	$2m$	$4m$	$15mn - 18m$

Table 2. Edge partition of graph of $NHPX[m,n]$ nanotubes based on degree sum of vertices lying at unit distance from end vertices of each edge.

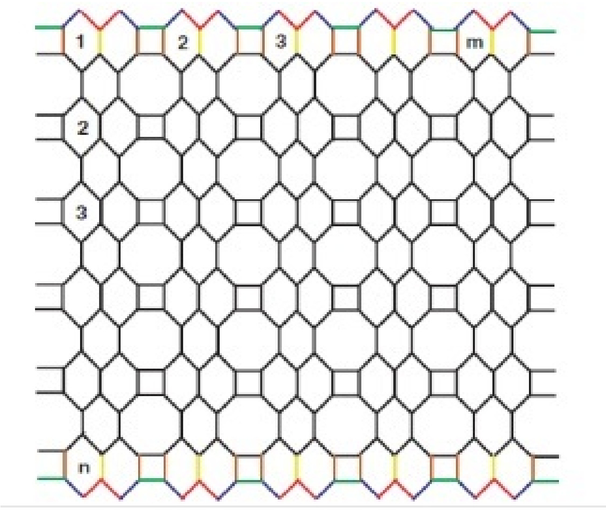

Figure 2. A graph of H-naphtalenic nanotube $NPHX[m,n]$ showing different partite sets based on the degree sum of neighbours of end vertices of each edge.

nanotube. In Figure 2, red colour shows the edges ab with $S_a = 6$ and $S_b = 7$, blue colour shows the type of edges ab with $S_a = 6$ and $S_b = 8$, green colour shows the type of edges ab with $S_a = S_b = 8$, yellow colour shows the type of edges ab with $S_a = 7$ and $S_b = 9$, brown colour shows the type of edges ab with $S_a = 8$ and $S_b = 9$ and black colour shows the partition having edges ab with $S_a = S_b = 9$.

In Table 2, cardinalities of such partite series of edge set of graph of $NHPX[m,n]$ nanotube are shown. In the following theorem, GA_2 index of $NHPX[m,n]$ nanotube and SK_3 index of $NHPX[m,n]$ nanotube is computed. □

Theorem 3.5. *Consider the graph of $NPHX[m,n]$ nanotube, then its GA_2 index is equal to*

$$GA_2(NPHX[m,n]) = \left(15n + \frac{26}{\sqrt{42}} + \frac{28}{\sqrt{48}} + \frac{16}{\sqrt{63}} + \frac{34}{\sqrt{72}} - 16\right) m.$$

Proof. We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Now by using the partition given in Table 2 we can apply the formula of GA_2 index to compute this index for $NPHX[m,n]$ nanotube.

$$GA_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}}.$$

$$\begin{aligned}GA_2(NPHX(n)) &= 4m\left(\frac{6+7}{2\sqrt{42}}\right)+4m\left(\frac{6+8}{2\sqrt{48}}\right)+2m\left(\frac{8+8}{2\sqrt{64}}\right)+2m\left(\frac{7+9}{2\sqrt{63}}\right)\\ &+4m\left(\frac{8+9}{2\sqrt{72}}\right)+(15mn-8m)\left(\frac{9+9}{2\sqrt{81}}\right)\\ &=\frac{26m}{\sqrt{42}}+\frac{28m}{\sqrt{48}}+2m+\frac{16m}{\sqrt{63}}+\frac{34m}{\sqrt{72}}+15mn-18m\\ &=\left(15n+\frac{26}{\sqrt{42}}+\frac{28}{\sqrt{48}}+\frac{16}{\sqrt{63}}+\frac{34}{\sqrt{72}}-16\right).\end{aligned}$$

□

Theorem 3.6. *Consider the graph of $NPHX[m,n]$ nanotube, then its SK_3 index is equal to*

$$SK_3(NPHX[m,n]) = (135n-42)\,m.$$

Proof. We use the edge partition of graph of $NPHX[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Now by using the partition given in Table 2 we can apply the formula of SK_3 index to compute this index for $NPHX[m,n]$ nanotube.

$$SK_3(G) = \sum_{u,v\in E(G)} \frac{S_G(u)+S_G(v)}{2}.$$

$$\begin{aligned}SK_3(NPHX(n)) &= 4m\left(\frac{6+7}{2}\right)+4m\left(\frac{6+8}{2}\right)+2m\left(\frac{8+8}{2}\right)+2m\left(\frac{7+9}{2}\right)+4m\left(\frac{8+9}{2}\right)\\ &+(15mn-8m)\left(\frac{9+9}{2}\right)\\ &=26m+28m+16m+34m+135mn-162m\\ &=(135n-42)\,m.\end{aligned}$$

3.2 Results for nanotubes coverd by C_4

In this section, we compute certain topological indices of nanotube covered only by C_4. The 2D-lattice of this family of nanotubes is a plane tiling of C_4. This tessellation of C_4 can either cover a cylinder or a torus. This family of nanotubes is denoted by $TUC_4[m,n]$, in which m is the number of squares in a row and n is the number of squares in a column as shown in Figure 4. A 3D representation of $TUC_4[m,n]$ nanotubes is depicted in Figure 3. There are three types of edges in 2D-lattice of $TUC_4[m,n]$ nanotube based on degrees of end vertices of each edge. Figure 3, explains such a partition of edges in which red coloured edges are the edges ab with $d_a = d_b = 3$, blue coloured edges are the edges ab with $d_a = 3$, $d_b = 4$ and black coloured edges are the edges ab with $d_a = d_b = 4$. Table 3 shows the number of edges in each partite set. □

Theorem 3.7. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its GA_1 index is equal to*

$$GA_1(TUC_4[m,n]) = \left(2n+\frac{7}{\sqrt{12}}-1\right)(m+1).$$

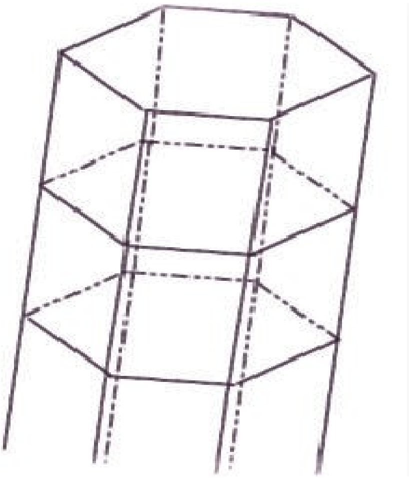

Figure 3. A $TUC_4[6,n]$ nanotube covered by C_4.

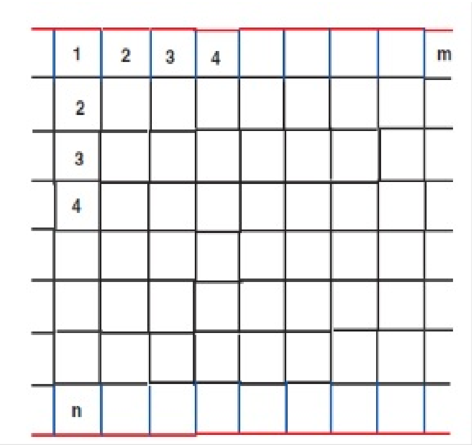

Figure 4. A graph of $TUC_4[m,n]$ nanotube showing the edge partition based on the degree of end vertices of each edge.

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the GA_1 index of $TUC_4[m,n]$ nanotube.

$$GA_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u)+d_G(v)}{2\sqrt{d_G(u).d_G(v)}}.$$

$$\begin{aligned} GA_1(TUC_4[m,n]) &= (2m+2)\left(\frac{3+3}{2\sqrt{9}}\right) + (2m+2)\left(\frac{3+4}{2\sqrt{12}}\right) \\ &+ (m+1)(2n-3)\left(\frac{4+4}{2\sqrt{16}}\right) \\ &= (2m+2) + (2m+2)\left(\frac{7}{2\sqrt{12}}\right) + (m+1)(2n-3) \end{aligned}$$

(d_a, d_b) where $u,v \in E(H)$	(3,3)	(3,4)	(4,4)
Number of edges	$(2m+2)$	$(2m+2)$	$(m+1)(2n-3)$

Table 3. Cardinalities of different partite sets based on degrees of end vertices of each edge of graph of $TUC_4[m,n]$ nanotube.

$$\begin{aligned}
&= 2mn + \left(\frac{7}{2\sqrt{12}}\right) - m + \left(\frac{7}{2\sqrt{12}}\right) - 1 \\
&= \left(2n + \frac{7}{\sqrt{12}} - 1\right) - m + \frac{7}{12} - 1 + 2n \\
&= \left(2n + \frac{7}{\sqrt{12}} - 1\right)(m+1).
\end{aligned}$$

□

Theorem 3.8. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its SK index is equal to*

$$SK(TUC_4[m,n]) = (8n+1)(m+1).$$

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the SK index of $TUC_4[m,n]$ nanotube.

$$SK(G) = \sum_{u,v \in E(G)} \frac{d_G(u) + d_G(v)}{2}.$$

$$\begin{aligned}
SK(TUC_4[m,n]) &= (2m+2)\left(\frac{3+3}{2}\right) + (2m+2)\left(\frac{3+4}{2}\right) + (m+1)(2n-3)\left(\frac{4+4}{2}\right) \\
&= 6m + 6 + 7m + 7 + (2mn - 3m + 2n - 3)4 \\
&= (8n+1)m + 8n + 1 \\
&= (8n+1)(m+1).
\end{aligned}$$

□

Theorem 3.9. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its SK_1 index is equal to*

$$SK_1(TUC_4[m,n]) = (16n-3)(m+1).$$

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the SK_1 index of $TUC_4[m,n]$ nanotube.

$$SK_1(G) = \sum_{u,v \in E(G)} \frac{d_G(u).d_G(v)}{2}.$$

$$\begin{aligned}SK_1\left(TUC_4\left[m,n\right]\right) &= \left(2m+2\right)\left(\frac{3\times 3}{2}\right)+\left(2m+2\right)\left(\frac{3\times 4}{2}\right)+\left(m+1\right)\left(2n-3\right)\left(\frac{4\times 4}{2}\right)\\ &= 9m+9+12m+12+\left(2mn-3m+2n-3\right)8\\ &= \left(16n-3\right)m+16n+1\\ &= \left(16n-3\right)\left(m+1\right).\end{aligned}$$

□

Theorem 3.10. *Consider the graph of $TUC_4[m,n]$ nanotubes, then its SK_2 index is equal to*

$$SK_2(TUC_4[m,n]) = \frac{1}{2}\left(64n-11\right)\left(m+1\right).$$

Proof. Consider the graph of $TUC_4[m,n]$. By using the edge partition based on the degrees of end vertices with respect to each edge on graph of $TUC_4[m,n]$ nanotube given in Table 3, we compute the SK_2 index of $TUC_4[m,n]$ nanotube.

$$SK_2(G) = \sum_{u,v\in E(G)}\left(\frac{d_G(u)+d_G(v)}{2}\right)^2.$$

$$\begin{aligned}SK_2(TUC_4[m,n])) &= \left(2m+2\right)\left(\frac{3+3}{2}\right)^2+\left(2m+2\right)\left(\frac{3+4}{2}\right)^2+\left(m+1\right)\left(2n-3\right)\left(\frac{4+4}{2}\right)^2\\ &= \left(2m+2\right)9+\left(2m+2\right)\left(\frac{49}{4}\right)+\left(2mn-3m+2n-3\right)16\\ &= \frac{1}{2}(64mn-11m+64n-11)\\ &= \frac{1}{2}\left(\left(64n-11\right)m+64n-11\right)\\ &= \frac{1}{2}\left(64n-11\right)\left(m+1\right).\end{aligned}$$

Now we compute GA_2 and SK_3 indices for two dimensional lattice of $TUC_4[m,n]$ nanotubes. There are five types of edges in the graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each, as shown in Figure 5, in which red coloured edges are the edge ab with $S_a = S_b = 7$, blue coloured edges are the edge ab with $S_a = 7$ and $S_b = 15$, green coloured edges are the edge ab with $S_a = S_b = 15$, yellow coloured edges are the edge ab with $S_a = 15$ and $S_b = 16$, and black coloured edges are the edge ab with $S_a = S_b = 16$. Table 4 shows the cardinalities of these partite sets.

□

Theorem 3.11. *Let $TUC_4[m,n]$ nanotube be a graph with $(m \geq 1, n \geq 4)$, then its GA_2 index is*

$$GA_2(TUC_4[m,n]) = \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right)\left(m+1\right).$$

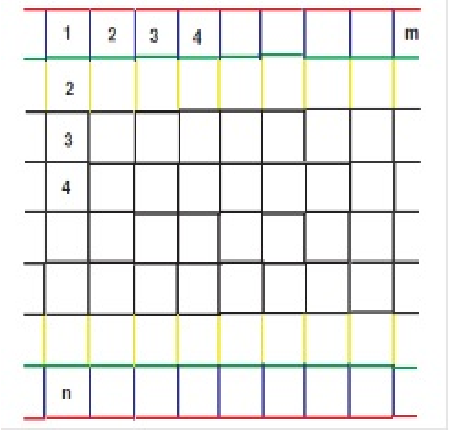

Figure 5. A graph of $TUC_4[m,n]$ nanotube showing the edge partition based on the degree sum of end vertices lying at unit distance from end vertices of each edge.

Table 4. Edge partition of graph of $TUC_4[m,n]$ nanotube based on degree sum of vertices lying at unit distance from end vertices of each edge.

(S_a, S_b) where $u,v \in E(H)$	(7,7)	(7,15)	(15,15)	(15,16)	(16,16)
Number of edges	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(2m+2)$	$(m+1)(2n-7)$

Proof. We use the edge partition of graph of $TUC_4[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge.

Now by using the partition given in Table 4 we can apply the formula of GA_2 index to compute this index for $TUC_4[m,n]$ nanotube.

$$GA_2(G) = \sum_{u,v \in E(G)} \frac{S_G(u) + S_G(v)}{2\sqrt{S_G(u).S_G(v)}}.$$

$$\begin{aligned} GA_2(TUC_4[m,n]) &= (2m+2)\left(\frac{7+7}{2\sqrt{49}}\right) + (2m+2)\left(\frac{7+15}{2\sqrt{105}}\right) + (2m+2)\left(\frac{15+15}{2\sqrt{225}}\right) \\ &+ (2m+2)\left(\frac{15+16}{2\sqrt{240}}\right) + (m+1)\,(2n-7)\left(\frac{16+16}{2\sqrt{256}}\right) \\ &= 2m+2+\frac{22m+22}{\sqrt{105}} + 2m+2+\frac{31m+31}{\sqrt{240}} + 2mn-7m+2n-7 \\ &= 2mn-3m+2n-3+\frac{22m+22}{\sqrt{105}}+\frac{31m+31}{\sqrt{240}} \\ &= \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right)m + \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right) \\ &= \left(2n-3+\frac{22}{\sqrt{105}}+\frac{31}{\sqrt{240}}\right)(m+1). \end{aligned}$$

□

Theorem 3.12. *Let $TUC_4[m,n]$ nanotube be a graph with $(m \geq 1, n \geq 4)$, then its SK_3 index is*

$$SK_3(TUC_4[m,n]) = (32n-15)(m+1).$$

Proof. We use the edge partition of graph of $TUC_4[m,n]$ nanotube based on the degree sum of vertices lying at unit distance from end vertices of each edge. Now by using the partition given in Table 4, we can apply the formula of GA_2 index to compute this index for $TUC_4[m,n]$ nanotube.

$$SK_3(G) = \sum_{u,v \in E(G)} \frac{S_G(u)+S_G(v)}{2}.$$

$$\begin{aligned} SK_3(TUC_4[m,n]) &= (2m+2)\left(\frac{7+7}{2}\right) + (2m+2)\left(\frac{7+15}{2}\right) + (2m+2)\left(\frac{15+15}{2}\right) \\ &+ (2m+2)\left(\frac{15+16}{2}\right) + (m+1)(2n-7)\left(\frac{16+16}{2}\right) \\ &= 14m+14+22m+22+30m+30+31+(2mn-7m+2n-7)16 \\ &= 32mn-15m+32n-15 \\ &= (32n-15)m+32n-15 \\ &= (32n-15)(m+1). \end{aligned}$$

□

Concluding Remarks: A generalized formula for geometric-arithmetic index (GA_1 index), SK index, SK_1 index, SK_2 index, SK_3 index, GA_2 index for H-naphtalenic nanotube and $TUC_4[m,n]$ nanotube is obtained without using a computer.

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Original Research Paper Economics

Chilli Cultivation in India and Karnataka: with Special Reference to Haveri District

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ABSTRACT

Chilli is one of the most valuable crops of India. Different varieties are grown for vegetables, spices, condiments, sauces and pickles. The crop is grown practically all over India. Among the most important states only for Andhra Pradesh, Maharashtra, Karnataka and Tamil Nadu account for three fourths of the total area. The other states having large areas under chillies are Madhya Pradesh, Punjab and Bihar. A small quantity of dry chilli is also exported. There is good scope for increasing its exports by pushing up production. Indian dry chillies are exported mainly to Srilanka, the USA, Canada, the UK, Saudi Arabia, Singapore, Malaysia and Germany, chillies are dry exported in different from fresh chillies, green chillies, chilli power and also as oleoresin. Dry chillies are grown in an area of 144707 hectares in Karnataka. The annual production of dry chillies is 230430 lakh tonnes. The average annual production per hectare in the State is 171 kgs. The chilli production in Karnataka is mainly rain-fed. Hence, the yield per hectare is low. The crop can be grown during all the seasons of the year.

KEYWORDS Chilli, Production, Yield

Introduction:

In this paper an attempt is made to know the importance of dry chilli in Indian Economy. By studying agro- climatic condition, soil, land preparation, harvesting, storage, fertilizer application, plant protection, quality standards, irrigation, commercial classification of chilli, grading of chilli, area and production of dry chilli, exports of dry chilli in India and Karnataka. The main thrust of analysis in this paper is to provide an overview of the cultivation, production and marketing of chillies in India and Karnataka and Haveri District in particular.

Importance of Chilli in India:

Indian agriculture is playing a very important role both in the internal and external trade of the country. "Agriculture products like tea, coffee, sugar, tobacco, spices, cashew nuts, dry chilli etc.," are the main items of our exports and constitute about 30 percent of our total exports. "Moreover, manufactured jute, cotton textiles and dry chilli also contribute another 20 and 27 percent of the total exports of the country". Thus, "nearly 77 percent of India's exports are originated from agricultural sector".

Chilli crop is raised for ripe dry chillies and green pads. The dried forms of the fruits of the genus capsicum, which entirely falls into three categories, dry chillies, capsicums and paprika. The term chillies are generally applied to the small fruited forms of several capsicum species. "The term capsicum is generally used to describe the somewhat larger fruited mild to moderately pungent forms. Paprika's are sweet or mildly pungent forms and primarily valued for it red colouring power."

Objectives of the Study

1. To study the area and production of dry chilli in India and Karnatraka.
2. To identify the marketing channel of dry chilli in Karnataka.
3. To analyse the area, production and yield of dry chilli in Haveri district.

Area and Production of Dry Chilli in India

In India, Chilli is cultivated in almost all the states. India is the largest producer chillies in the world. In India chilli is cultivated in almost all the states. The area under chillies and its production is represented in table-1.

Table – 1: Area and Production of Dry Chilli in India 1998-99 to 2006-07

Sl. No.	Year	Area in Hectares	Per cent Increase or decrease over previous year	Production in Tonnes	Per cent Increase or decrease over previous year	Yield Kgs/hectare
1	1998-1999	753100	-	5201776	-	691
2	1999-2000	883700	17.34	5797872	11.46	656
3	2000-2001	944200	6.85	8648872	49.17	916
4	2001-2002	881290	-6.66	9949764	15.04	1129
5	2002-2003	831630	-5.63	8457677	-15.00	1017
6	2003-2004	858784	3.27	10219529	20.83	1190
7	2004-2005	859200	0.05	10851696	6.19	1263
8	2005-2006	867783	1.00	10140000	-6.56	1168
9	2006-2007	763000	-12.07	1242000	-87.75	1628
10	2007-2008	805000	5.50	1292000	4.03	1605
11	2008-2009	779000	-3.23	1269000	-1.78	1629
12	2009-2010	767000	-1.54	1202000	-5.28	1567
13	2010-2011	792000	3.26	1223000	1.75	1544
14	2011-2012	804000	1.52	1276000	4.33	1587
15	2012-2013	794000	-1.24	1304000	2.19	1642

Source:
1. Agricultural Situation in India.
2. FAO Year Book Annual Production 1998-99 to 2012-2013. ww.fao.org.

Area:
The total area under cultivation of dry chilli rose from 753100 hectares in 1998-99 to 883700 hectares in 1999-2000 and further to a record level of 944200 hectares in 2000-01. The subsequent period of 2 years experienced a decline in the total area under dry chilli, which came down to 881290 hectares in 2001-02 and further to a low level of 831630 hectares in 2002-03. Fluctuating trend in the area under dry chilli is noticed again during the next 5 years. The area under cultivation of dry chillies rose marginaly to 858784 hectares in 2003-04 compared to the previous year. A sharp increase in the area under cultivation from 859200 hectares in 2004-05. A decline in the total area under dry chilli, which came down to 794000 hectares in 2012-13. The details are presented in table-1.

Production:
Fluctuating trends in the production of dry chilli in India are discernible during the decade from 1998-99 to 2006-07. Table-1 production of dry chilli came down to 8457677 tonnes in 2002-2003 but showed a revival for the next two years. The production of dry chilli increased to 10219529 tonnes in 2003-04 and further to a record level of 10851696 tonnes in 2004-05. A decline in the total production of dry chilli, which came down to1304000 tonnes in 2012-2013.

Yield:
The figures of yield per the hectare of dry chilli in India reveal the same significant trends during the period from 1998-99 to 2006-07. A greater degree of stability in the yield of dry chillies per hectare is discernible though with some milled amount of fluctuations during the decade. The yield per hectare of dry chillies declined from 690 Kg. in 1998-99 to 656 Kg. in per hectare in 1999-00 but chillies steeply to 916 Kg. per hectare in 2000-01 to 1129 Kg. per hectare in 2001-02. The next years experienced some decline from 1017 kg in 2002-03 but rose steeply to 1190 kg., in 2002-03 but dry chilli steeply to 1190 Kg. per hectare in 2003-04. With some fluctuations in the yield per hectare during the subsequent 5 years there was a record rise to 1643 Kg. per hectare in 2012-2013. It is clear from table-1 that there has been a positive growth trend in all three parameters of growth in the area, production and yield of dry chilli during the period from 1998-99 to 2012-2013.

Export of Dry Chillies in India
The potential for increasing exports of whole chillies, chilli powder and crushed chillies in consumer packs is very high. But consumers in importing countries insist on 'clean spices' and to meet this challenge. Indian producers and exporters should make every effort to prevent contamination from external sources during harvesting, post harvest, handling, processing and storage. "This can be achieved only through an integrated approach with the collective efforts of farmers, processors and traders." Improved quality and productivity of Indian chillies will help promote exports and effectively meet the competition from other producing and exporting countries. "Conformance to the quality requirements of the buying countries, meeting the consumer's expectations and ability to maintain price competitiveness are the key factors which determine our survival in the international market."

Export trends of dry chillies during the last 9 years show some significant trends. Year after year fluctuations in the exports of dry chillies are noticed during the last 9 years from 2000-01 to 2008-2009. In spite of the fluctuations, both in terms of quantity and the value of export has registered an upward trend as could be seen in Table-2.

Table-2: Export of Dry Chillies in India

Sl. No.	Years	Total Production (in Tonnes)	Total Quantity Export (in tonnes)	Percentage of Exports	Value (Rs.in lakhs)`
1	2000-01	8648872	62447.68	0.72	22,973.30
2	2001-02	9949764	65000	0.65	25,000.00
3	2002-03	8457677	81022	0.96	31,514.00
4	2003-04	10219529	86575.34	0.85	36,687.34
5	2004-05	10851696	138000	1.27	49,900.00
6	2005-2006	10140000	113174	1.12	40300.51
7	2006-2007	1242000	148500	11.96	80775.00
8	2007-2008	1292000	209000	16.18	109750.00
9	2008-2009	1269000	188000	14.81	108095.00

Source:
1) KARVY Commodities Research @ Karvv.com
2) Spices Board of India

United States of America is the major importer of dry chillies from India which contributes 24 percent to the total exports from India. Srilanka stand second with 24 percent followed by Bangladesh (13 percent), Malaysia (6 percent) and others (28 percent).

The upswing in the production of dry chilli crop last year and a consequent availability of large exportable surplus in the country when the crop in other major producing countries declined have resulted in a boom for dry chilli exports touching an all time high of an estimated 138000 tonnes valued at over Rs. 49,900.00 lakhs in 2004-05. India started exporting dry chilli in 1960-61 with 8364 tonnes valued at Rs. 176 crore, was in 2003-04 with 86575.34 tonnes valued at Rs. 36,687.81 lakhs in 2002-03, it was 81022 tonnes valued at Rs.31514 lakhs. After 2001-02 India export performance was excellent, higher international and domestic demand can further push the exports.

India exports dry chilli in the different processed forms like dry chilli powder dried chillies, pickled chillies etc and it is mainly exported to USA, Srilanka, Bangladesh, the Middle East and the Far East. There is a lot of voltage in the Indian dry chilli exports by dominating in the international markets and processed dry chilli can bring big boost to the prices, which can avail to higher exports. Among the total exports dry chilli contributes a majority of 72 percent to the total exports from India, followed by chilli powder with 27 percent and chilli seed (1 percent).

Area under Chilli Production and Yield per Hectare in Karnataka
The decline in the area under dry chillies from 159364 hectares in 2000-01 and 151377 hectares in 2002-03 and the subsequent period experienced a considerable stability of area under dry chillies from 1998-99 to 2004-05. Fluctuations in the dry chilli covered area in Karnataka during the last seven years are observed from table-3.

Table-3: Area and Production of Dry Chillies in Karnataka State (1998 –99 to 2012-2013)

Sl. No.	Year	Area (in Hectares)	Percentage Increase or Decrease Over Previous Year	Production (in tonnes)	Percentage Increase or Decrease As Per Previous Year	Yield kg /per Hectare
1	1998-99	170375	-	540648	-	317
2	1999-00	186901	8.84	457411	-18.20	245
3	2000-01	159364	-17.28	178285	-56.56	112

4	2001-02	171532	7.09	185901	4.10	108
5	2002-03	151377	-13.31	214320	13.26	142
6	2003-04	101289	-49.45	118345	-81.10	117
7	2004-05	144707	30.00	230430	48.64	159
8	2005-06	134703	-7.43	210210	-9.62	156
9	2006-07	121532	-10.84	129100	-62.83	106
10	2007-08	122633	0.90	168211	23.25	137
11	2008-09	122000	-0.52	135100	-24.51	111
12	2009-10	138000	11.59	138200	2.24	100
13	2010-11	113800	-21.27	122900	-12.45	108
14	2011-12	805000	85.86	127600	3.68	16
15	2012-13	794000	-1.39	130400	2.15	317

Sources: Horticultural crop statistics of Karnataka State at a Glance and Krishipethe, Agricultural Marketing Board, Bangalore

The production of dry chillies during the nine year period from 1998-99 to 2006-07 reveals a greater degree of stability. The production of dry chillies in Karnataka increase from 540648 tonnes in 1998-99. There has been decrease in 457411 tonnes in 1999-2000 and 178285 tonnes in 2000-01. There has been considerable increase to 185901, 214320 and 2748.51 tonnes in the years 2001-02, 2002-03 and 2004-05 respectively. The again decrease in 212994 tonnes in the year 2003-04.

The yield per hectare of dry chillies in Karnataka fluctuated during the first two years. It yields from 317 kg per hectare in 1998-99 but decline to 245 kg per hectare in 1999-2000, 112 kg in 2000-01 and 108 kg in 2001-02. The yield per hectare shows increase in the subsequent period.

Marketing of Dry Chillies

Marketing of dry chillies is carried on through the village merchants and commission agents. Farming uses their own vehicles in transporting their produce from the fields to the markets. Other hires transport such as trucks and tractors. Transport facilities are mostly owned by the intermediaries and use them to transport the produce from villages to the marketing centers. Grading of dry chillies extensively and the regulated markets in almost all the taluka places also provide grading facilities. The grading of dry chillies in regulated markets is done on the basis of variety, size of pods, colour, taste, moisture and seed content. There should be uniformity in the colour of the fruits and it should not vary from bag to bag within the consignment.

Comparison of Average Yield per Hectare with National Average in Dry Chillies (1998-99 to 2004-05)

The dry chilli was decreasing 171 kg for Karnataka State during the same average same period and the net difference was 805.42 kg for dry chillies. The factor responsible for this phenomenon was the poor yield caused by adverse weather, pests and diseases.

The year wise distribution of the area under dry chilli in the district also showed irregularities. On the whole it could be found that larger portion of the dry chilli come from Haveri districts is accounted for 23.04 percent during the decade of study.

Table – 4: Comparison of Karnataka's average yield per hectare with national average in Dry Chilli (1998-99 to 2012-13)

Sl. No.	Year	Dry Chillies		
		Average yield in India (In Kg.)	Average in yield in Karnataka (In Kg.)	Net Difference
1	1998-1999	664	317	347
2	1999-2000	656	244	412
3	2000-2001	916	111	805
4	2001-2002	1129	108	1021
5	2002-2003	1017	141	876
6	2003-2004	1190	117	1073
7	2004-2005	1263	159	1104
8	2005-2006	1551	146	1405
9	2006-2007	1627	1151	476
10	2007-2008	1611	1161	450
11	2008-2009	1630	1162	468
12	2009-2010	1568	1048	520
13	2010-2011	1544	1136	408
14	2011-2012	1586	1115	471
15	2012-2013	1643	1124	519

Sources:
1) Horticultural crop statistic of Karnataka State at a Glance.
2) Chilli Agri-Export Zone in Bangalore.

Haveri headed the group with an average percentage of 33.88 followed by Davanagere (13.18) and Tumkur (12.32). Together only these three districts, contributed 59.38 percent of the total chilli area in the State during the decade as compared to dry chilli Dharwad district is an average percentage of 37.58 followed by Haveri (23.04 percent) and Gadag (9.36 percent) Together only these three districts, contributed 69.98 percent of the total dry chilli area in the State during the decade. The year wise break-up presented no different picture.

Area Production and Yield of Dry Chillies in Haveri District

Haveri district has the maximum area under the dry chillies crop in Karnataka and it also tops the list of district wise production of dry chillies in the State. Haveri is one of the few important districts growing dry chillies in India. The annual figures of area, production and yield of dry chillies are provided in Table-5.

Table – 5: Area, production and yield of Dry chillies in Haveri District

Sl. No.	Year	Area (in Hectares)	Percentage Increase or decrease over previous year	Production (in Tonnes)	Percentage Increase or decrease over previous year	Average Yield per hectare
1	1998-1999	27145	--	133033	--	490
2	1999-2000	44610	+64.33	147983	+11.23	331
3	2000-2001	36137	-18.99	48472	-67.24	134
4	2001-2002	40304	+11.53	33162	-31.59	082
5	2002-2003	38369	-4.80	99840	+201.06	260
6	2003-2004	26828	-30.07	26828	-73.13	147
7	2004-2005	33274	+24.02	48811	+81.94	147
8	2005-2006	43129	+29.62	87475	+79.21	202.82
Average		35238.14	--	76875.57	--	227.29

Source :
1) Horticultural Crop Statistic of Karnataka State at a Glance
2) District Statistical Office of Haveri

The production was also decreased from 48472 tonnes in year 2000-01. Then, again increased area about 40304 hectares in year 2001-02, but production of dry chilli is decreased from 33162 tonnes during the year 2001-02.

Table- 6: Share of Haveri District in Dry Chilli in Karnataka State (1998-1999 to 2004-2005)

Sl. No.	Year	Area under Dry Chilli (in hectares)			Production of Dry Chilli (in tonnes)		
		Karnataka State	Haveri District	Percentage Share of Haveri District	Karnataka State	Haveri District	Percentage Share of Haveri District
1	1998-1999	170375	27145	15.93	540648	133033	24.61
2	1999-2000	186901	44610	23.87	457411	147983	32.35
3	2000-2001	159364	36137	22.68	178285	48472	27.19
4	2001-2002	171532	40304	23.49	185901	33162	17.84
5	2002-2003	151377	38369	25.35	214320	99840	46.58
6	2003-2004	101289	26828	26.49	118345	26828	22.67
7	2004-2005	144707	33274	22.99	230430	48811	21.19
Average		155077.86	35238.14	22.72	275048.57	76875.57	27.95

Source:
1) Horticultural Crop Statistic of Karnataka State at a Glance
2) District Statistical Office of Haveri

The dry chilli area is declined for the 38369 hectares in 2002-03 but production of dry chilli more was 99840 in the same year. Further, there was an increase in area from 26828 hectares in 2003-04 to 33274 hectares in 2004-05, but production was declined for the 26828 tonnes in 2003-04 in case of year 2004-05 production is increase in 48811 tonnes over the previous year. But again increase in area is 33274 hectares and 43129 hectares in 2004-05 and 2005-06 years. The production was also increasing 48811 tonnes and 87475 tonnes as a same during period.

Major Findings

1. Chilli growing becomes the top priority in Savanur taluka nearly 32.70 percent of the land is suitable for Chilli cultivation. As results, there has been much increase in production every year.
2. Chilli has been growing during Kharif season and 75 percent of the Chilli area depends on rainfall and 25 percent area is being irrigated.
3. Chilli production and cultivation also has been increased due to adoption of high yielding varieties of seeds use of technology, fertilizer, monure and scientific inputs.
4. The Chilli is a brought under cultivation both in irrigated and non-irrigated regions.
5. The average annual area under cultivation of chilli in India is is increase to 858843.42 hectares.
6. The average annual production of dry chilli in India is 7778169.42 tonnes.
7. The average annual yield per hectare of dry chilli in India is 976.42 Kgs.
8. The average annual area of cultivation of dry chilli in Karnataka is 155077.86 hectares.
9. Average annual production of dry chilli in Karnataka is 275048.57 tonnes.
10. Average annual yield per hectare of dry chilli in Karnataka is 171kg.

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IOSR Journal of Mathematics (IOSR-JM)
e-ISSN: 2278-5728, p-ISSN: 2319-765X. Volume 12, Issue 2 Ver. IV (Mar. - Apr. 2016), PP 36-39
www.iosrjournals.org

Correlation between the Arithmetic-Geometric Indices of n-Heptane Alkane Isomers

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Abstract:*In this paper, the correlation abilities of nine vertex-degree-based AG (Arithmetic-Geometric) indices occurring in the physico-chemical properties of boiling point , density and refractive index of n-heptane alkane isomers is presented.*

Keywords:*Arithmetic-Geometric Index, graph theory, n-heptane alkane isomers.*

I. Introduction

Let G be a simple graph with n vertices and m edges, with vertex set $V(G)=\{v_1,v_2,\ldots..,v_n\}$ and edge set E(G). The edge connecting the vertices v_i and v_j will be denoted by v_iv_j. The degree of the vertex v_i, denoted by d_i, is the number of first neighbors of v_i in the underlying graph.

A topological index is a structural descriptor (derived from molecular graph) that represents an efficient way to express in a numerical form the size, shape, cyclicity and branching. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity[5].

II. Arithmetic-Geometric Index

One of the important degree based topological indices is Arithmetic-Geometric (AG) index of G

$$: AG(G)= \sum_{uv\in E(G)} \frac{du+dv}{2\sqrt{du.dv}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

Where, AG index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v. where du (or dv) denote the degree of the vertex u (or v)[6,7,8].

III. Data Sources

Boiling point , Density and Refractive index of n-Heptane alkane isomers are taken from Lecture 6(Structural Isomers).

IV. Figures and Tables

Table1. The values of Boiling point , Density , Refractive index and AG index of n-Heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Boiling point (^{0}C) Y_1	Density(g/cm^3)Y_2	RefractiveIndexY_3	AG(G)
I.	Heptane	98	0.684	1.3878	6.3034
II.	2-methylhexane	90	0.677	1.3848	6.3367
III.	3-methylhexane	92	0.686	1.3887	6.3365
IV.	2,2-dimethylpentane	79	0.674	1.3822	6.3713
V.	3,3-dimethylpentane	86	0.694	1.3909	6.3713
VI.	2,3-dimethylpentane	90	0.695	1.3919	6.3700
VII.	2,4-dimethylpentane	81	0.673	1.3815	6.3700
VIII.	3-ethylpentane	94	0.698	1.3934	6.3367
IX.	2,2,3-trimethylbutane	81	0.690	1.3894	6.4047

Table2. Comparison between experimental and predicted values of boiling point with respect to n-heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Experimental boiling point (^{0}C) Y_1	Predicted boiling point(^{0}C) Y_1^1
I.	Heptane	98	97.2523
II.	2-methylhexane	90	91.282
III.	3-methylhexane	92	91.3179
IV.	2,2-dimethylpentane	79	85.0786

V.	3,3-dimethylpentane	86	85.0786
VI.	2,3-dimethylpentane	90	85.3117
VII.	2,4-dimethylpentane	81	85.3117
VIII.	3-ethylpentane	94	91.282
IX.	2,2,3-trimethylbutane	81	79.0904

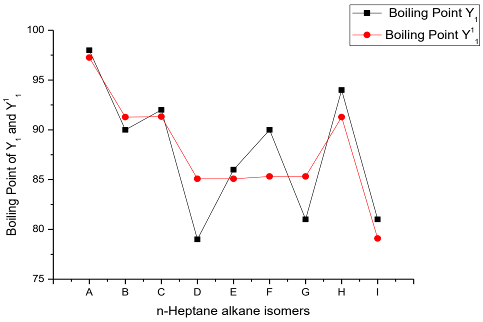

Figure1. The graph showing the n-Heptane alkane isomers versus Boiling point Y_1 and Y_1^1 values.

Table3. Comparison between experimental and predicted values of Density with respect to n-heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	ExperimentalDensity(g/cm^3)Y_2	Predicted Density(g/cm^3)Y_2^1
I.	Heptane	0.684	0.687
II.	2-methylhexane	0.677	0.686
III.	3-methylhexane	0.686	0.686
IV.	2,2-dimethylpentane	0.674	0.685
V.	3,3-dimethylpentane	0.694	0.685
VI.	2,3-dimethylpentane	0.695	0.685
VII.	2,4-dimethylpentane	0.673	0.686
VIII.	3-ethylpentane	0.698	0.686
IX.	2,2,3-trimethylbutane	0.690	0.683

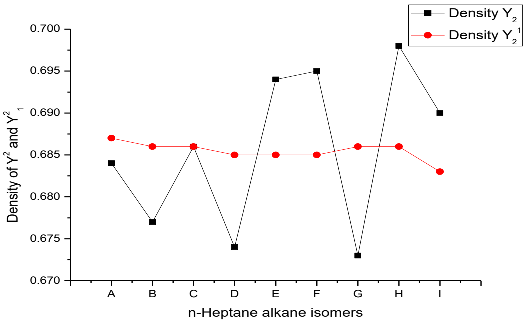

Figure2 The graph showing the n-Heptane alkane isomers versus Density Y_2 and Y_2^1 values.

Table4. Comparison between experimental and predicted values of Refractive index with respect to n-heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Experimental RefractiveIndexY_3	PredictedRefractiveIndexY_3^1
I.	Heptane	1.3878	1.3921
II.	2-methylhexane	1.3848	1.3895
III.	3-methylhexane	1.3887	1.3895
IV.	2,2-dimethylpentane	1.3822	1.3867
V.	3,3-dimethylpentane	1.3909	1.3867
VI.	2,3-dimethylpentane	1.3919	1.3868
VII.	2,4-dimethylpentane	1.3815	1.3868
VIII.	3-ethylpentane	1.3934	1.3895
IX.	2,2,3-trimethylbutane	1.3894	1.3841

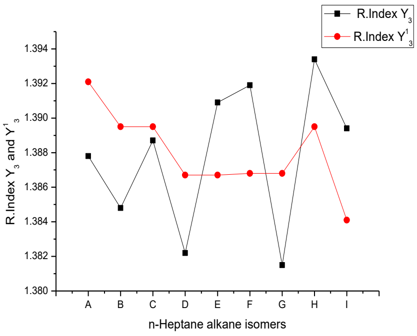

Figure3. The graph showing the n-Heptane alkane isomers versus Refractive index Y_3 andY_3^1 values.

Table5. Comparison between predicted values of Refractive index and Density with respect to n-heptane alkane isomers.

S.No.	C_7H_{16} alkane isomers name	Y_3^1	Y_2^1
I.	Heptane	1.3921	0.687
II.	2-methylhexane	1.3895	0.686
III.	3-methylhexane	1.3895	0.686
IV.	2,2-dimethylpentane	1.3867	0.685
V.	3,3-dimethylpentane	1.3867	0.685
VI.	2,3-dimethylpentane	1.3868	0.685
VII.	2,4-dimethylpentane	1.3868	0.686
VIII.	3-ethylpentane	1.3895	0.686
IX.	2,2,3-trimethylbutane	1.3841	0.683

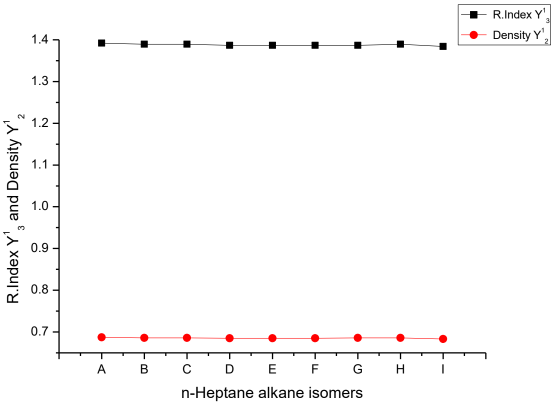

Figure4. The graph showing the n-Heptane alkane isomers versus predicted Refractive index (Y_3^1) and Density (Y_2^1) values.

V. Conclusion

Fig.1.n-Heptane alkane isomers are considered here to evaluate the correlation of boilingpoint and a comparison with the experimental value is carried out. Y_1 is the experimental boiling point and Y_1^1 is the boiling point determined using AG index. It can be seen that the both compound values (Y_1 and Y_1^1) are near to each other.

The above observation shows that the AG index derived can be used to determine the boiling point of n-heptane alkane isomers.

Fig.2: n-Heptane alkane isomers are considered here to evaluate the correlation of density and a comparison with the experimental value is carried out. Y_2 is the experimental density and Y_2^1 is the density determined using AG index. It can be seen that the both compound values (Y_2 and Y_2^1) are near to each other.

The above observation shows that the AG index derived can be used to determine the density of n-heptane alkane isomers.

Fig.3: n-Heptane alkane isomers are considered here to evaluate the correlation of refractive index and a comparison with the experimental value is carried out. Y_3 is the experimental refractive index and Y_3^1 is the refractive index determined using AG index. It can be seen that the both compound values (Y_3 and Y_3^1) are near to each other.

The above observation shows that the AG index derived can be used to determine the refractive index of n-heptane alkane isomers.

Fig.4: n-Heptane alkane isomers are considered here to evaluate the correlation of refractive index and a comparison with the density value is carried out. Y_3^1 is the refractive index and Y_2^1 is the density determined using AG index.It can be seen that the both compound values (Y_3^1 and Y_2^1) difference is nearly 0.7.

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JAMAL ACADEMIC RESEARCH JOURNAL: AN INTERDISCIPLINARY
Special Issue(February 2016), PP: 235-238
ISSN 0973 - 0303

DEGREE BASED TOPOLOGICAL INDICES OF n-HEPTANE ISOMERS

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Abstract

A graph$G = (V(G), E(G))$ consists of the vertex set V(G) and the edge set E(G) such that each edge e in E is assigned an unordered pair of vertices (u, v), called the end vertices of e. The skeleton of an organic molecule (usually, of a hydrocarbon) represents simple graph. Thus the vertices of molecular graph represent the carbon atoms, and edges the carbon-carbon bonds. In molecular graph we have many topological indices. In this paper, we are computing ABC index, GA index, AG index of n-heptane isomers.

Keywords: Graph, Molecular graph, ABC index, GA index, AG index.

2010 AMS Classification:

1 Introduction

Let G be a molecular graph. The vertex-set and edge set of G denoted by V(G) and E(G) respectively. The number of vertices of G, adjacent to a given vertex v, is the degree of this vertex and is denoted by d_v(G) or dv. The concept of degree in graph theory is closely related to valence in chemistry [2].chemical graphs are mathematical objects that represent chemical compounds.

A topological index is a structural descriptor (derived from molecular graph) that represents an efficient way to express in a numerical form the size, shape, cyclicity and branching. The topological indices of molecular graphs are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity[4].

Atom-Bond connectivity index: The atom-bond connectivity index, (ABC index),first proposed by Ernesto Estrada in 1998. Estrada is a Cuban mathematician born in 1996. He is currently a professor and chair in complexity sciences at the university of Strathclyde in Glasgow,Scotland . The ABC index is a new topological index that has proven to be a valuable predictive index in the study of the heat of formation in alkanes [3]. For those who may not be familiar with alkanes, these are any of the series of saturated hydrocarbons having the general formula CnH_{2n+2}, including methane, ethane and propane.

The ABC index comes from the connectivity index, which was introduced in 1975 by Milan Randic, however, the connectivity index deals with molecular branching, Estrada wanted to take into account the many physicochemical properties that are not dependent on branching, thus, the ABC index was born.

The ABC index is defined as follows,

$ABC(G)=\sum_{uv\in E(G)} \sqrt{\frac{du+dv-2}{du.dv}}$

Where the summation goes over all the edges of G, du and dv are the degrees of the terminal vertices u and v of edges uv and E(G) is the set of edges of G with cardinality m=$|E(G)|$

Geometric-arithmetic Index:

Another recently conceived vertex-degree-based topological index utilizes the difference between the geometric and arithmetic means, and is defined as

GA(G)= $\sum_{uv\in E(G)}\frac{2\sqrt{du.dv}}{du+dv}$

Where, of course, $\sqrt{du.dv}$ and $\frac{du+dv}{2}$ are the geometric and arithmetic means, respectively, of the degrees of the end-vertices of an edge.Recall that the former is always less than or equal to the later.The index was invented by Vukicevic and Furtula and was named "geometric-arithmetic index"[1].

Arithmetic-geometric Index:

One of important connectivity topological indices is Arithmetic-Geometric (AG) index of G

AG(G)=$\sum_{uv\in E(G)}\frac{du+dv}{2\sqrt{du.dv}}$

Where, AG index is considered for distinct vertices.

The above equation is the sum of the ratio of the Arithmetic mean and Geometric mean of u and v. where du (or dv) denote the degree of the vertex u (or v)[5,6,7].

There are nine different structural isomers. Their physical properties are different showing they are, in fact, distinct structures

C_7H_{16}alkane isomers name	**Boiling point (^{0}C)**	**Density (g/cm^3)**	**Refractive Index**
Heptane	98	0.684	1.3878
2-methylhexane	90	0.677	1.3848
3-methylhexane	92	0.686	1.3887
2,2-dimethylpentane	79	0.674	1.3822
3,3-dimethylpentane	86	0.694	1.3909
2,3-dimethylpentane	90	0.695	1.3919
2,4-dimethylpentane	81	0.673	1.3815
3-ethylpentane	94	0.698	1.3934
2,2,3-trimethylbutane	81	0.690	1.3894

2 Main Results and Discussion

There are nine different structural isomers, their different topological indices shown below.

S.No.	**C_7H_{16}alkane isomers name**	**AG(G)**	**GA(G)**	**ABC(G)**
I	Heptane	6.3034	5.8856	4.2426
II	2-methylhexane	6.3367	5.6545	4.3316
III	3-methylhexane	6.3365	5.7111	4.1449
IV	2,2-dimethylpentane	6.3713	5.2856	4.7193
V	3,3-dimethylpentane	6.3713	5.3712	4.7792
VI	2,3-dimethylpentane	6.3700	5.5205	4.5265
VII	2,4-dimethylpentane	6.3700	5.4235	4.6820
VIII	3-ethylpentane	6.3367	5.7676	4.2426
IX	2,2,3-trimethylbutane	6.4047	5.1217	4.8764

Fig.1. The graph shows the plot of different values of n-heptane alkane isomers versus the n-heptane alkane isomers.

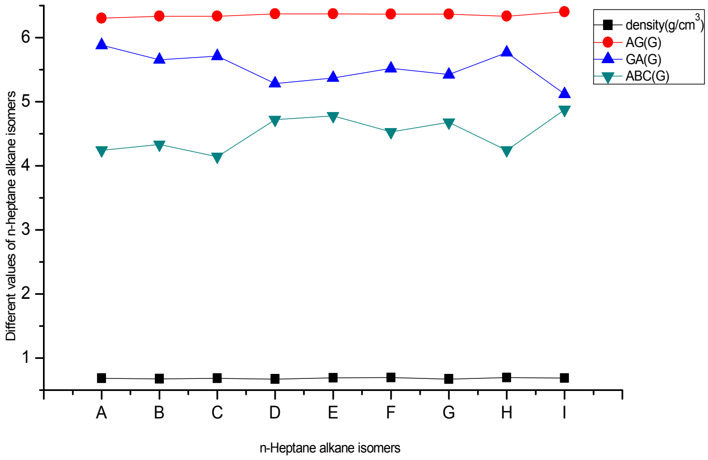

Figure 1

Fig.2. The graph shows the plot of different index values of n-heptane alkane isomers versus the n-heptane alkane isomers.

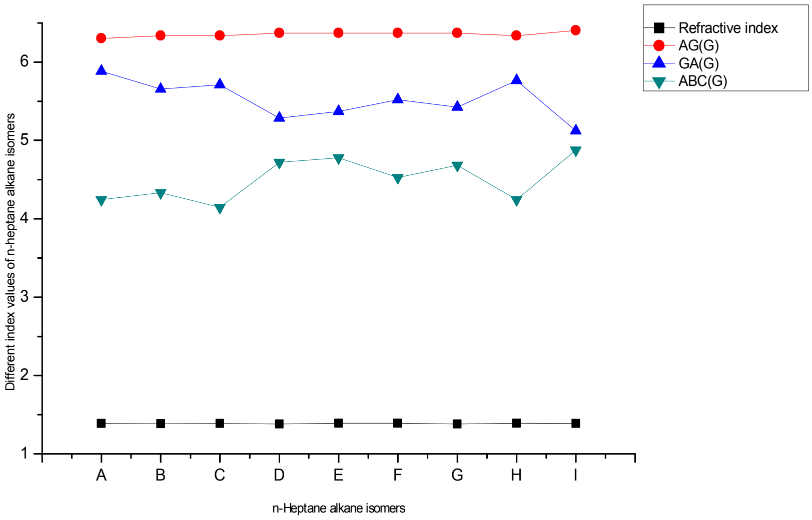

Figure 2

Fig.3. The graph shows the plot of different index and boiling point values of n-heptane alkane isomers versus the n-heptane alkane isomers.
A) Heptane, B) 2-methylhexane, C) 3-methylhexane, D) 2,2-dimethylpentane, E) 3,3-dimethylpentane, F) 2,3-dimethylpentane, G) 2,4-dimethylpentane, H) 3-ethylpentane, I) 2,2,3-trimethylbutane.

3 Conclusion

The topological indices are determined for some members of isomers of n-heptane and it is observed thatAG(G) $>$ GA(G) $>$ ABC(G).

Fig.1: The variation with respect to density,AG (G), GA(G) and ABC(G) are plotted.As can be seen from the graph, density and AG(G) variation remaining fairly constant for all the n-heptane alkane isomers.However the variation of GA(G) and ABC(G) across the

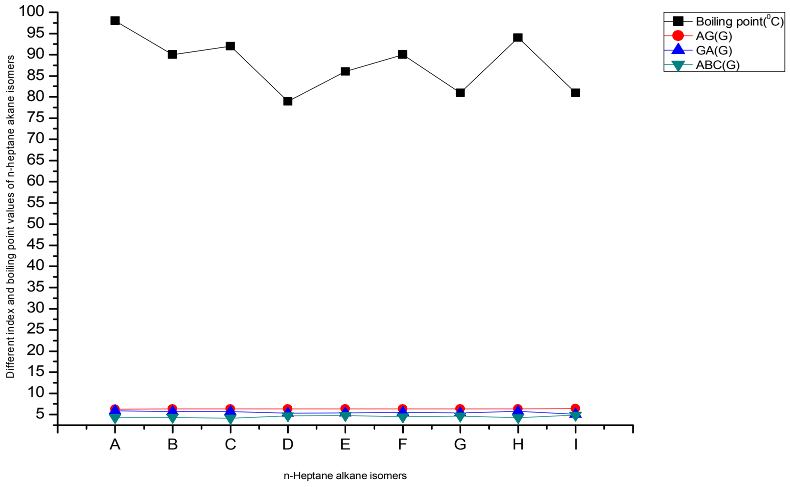

Figure 3

n-heptane alkane isomers is significant.The AG(G) value is very high and the density value is very low across the n-heptane alkane isomers.

Fig.2: The variation with respect to refractive index, AG(G),GA(G) and ABC(G) are plotted. As can be seen from the graph, refractive index and AG(G) variation remaining fairly constant for all the n-heptane alkane isomers. However the variation of GA(G) and ABC(G) across the n-heptane alkane isomers is significant. The AG(G) value is very high and the refractive index value is very low across the n-heptane alkane isomers.

Fig.3: The variation with respect to boiling point, AG(G),GA(G) and ABC(G) are plotted. As can be seen from the graph, the AG(G),GA(G) and ABC(G) variation remain almost constant for all the n-heptane alkane isomers.These values are very low. However the boiling point variation is high and its values are high.

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ASSESSMENT OF SEASONAL VARIATIONS IN WATER QUALITY OF MUDHOL TALUKA IN BAGALKOT DISTRICT, KARNATAKA INDIA .

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Abstract: Assessment of seasonal changes in surface water quality is an important aspect for evaluating temporal variations of water pollution due to natural or anthropogenic inputs of point and non-point sources. In this study, surface water quality data for 7 physical and chemical parameters collected from 50 monitoring stations in a water of Mudhol taluka of Bagalkot district, Karnataka were analyzed. The principal component analysis technique was employed to evaluate the seasonal variations of water quality parameters, while the principal factor analysis technique was used to extract the parameters that are most important in assessing seasonal variations of water quality. Analysis shows that a parameter that is most important in contributing to water quality variation for one season may not be important for another season except for DOC and electrical conductance, which were always the most important parameters in contributing to water quality variations for all four seasons

Introduction

Water is the most vital resources for all kinds of life on this planet. Water is one of the nature’s most important gifts to mankind. It is essential and most precious commodity for life. Rivers are vital and vulnerable freshwater systems and are essential for the sustenance of all life. Pollution of surface water with toxic chemicals and eutro-phication of rivers and lakes with excess nutrients are of great environmental concern worldwide. Agricultural, Indus-trial, and urban activities are considered as being major sources of chemicals and nutrients to aquatic ecosystems, while atmospheric deposition could be an important source to certain constituents such as mercury and nitrogen. The concentrations of toxic chemicals and biologically available nutrients in excess can lead to diverse problems such as toxic algal blooms, loss of oxygen, fish kills, loss of biodiversity, and loss of aquatic plant beds and coal reefs [1]. Nutrient enrichment seriously degrades aquatic ecosystems and impairs the use of water for drinking, industry, agriculture, and recreation and for other purposes. The modern civilization, urbanization and prolonged discharge of industrial effluents, domestic sewage and solid waste dump cause the water to became polluted. Wild and domestic animals using same drinking water can also contaminate the water through direct defection and urination [2]. The modern civilization, urbanization and prolonged discharge of industrial effluents, domestic sewage and solid waste dump cause the water to became polluted. Wild and domestic animals using same

drinking water can also contaminate the water through direct defection and urination [3]. Rivers are considered as vital and vulnerable freshwater ecosystems that are important for the sustenance of all life. Untreated discharge of pollutants to a water resource system from domestic sources, storm water discharges, industrial wastewaters, agricultural runoff and the other sources, all can have short term and long term significant effects on the quality of a river system[4]. The physico-chemical parameters useful for water quality assessment are determined by the presence of both organic and inorganic compounds that are either suspended or dissolved in water. At the same time, water quality characteristics of aquatic environment arise from a multitude of physical, chemical and biological interactions [5]. While some of these compounds are toxic to the ecosystem, some are providing nutrients to aquatic organisms and others are responsible for the aesthetics of the water body[6]. Human activities are a major factor determining the quality of the surface and ground water through atmospheric pollution, effluent discharges, use of agricultural chemicals, eroded soils and land use [7]. These land use changes increase the amount of impervious surface resulting in storm runoff events that negatively affect stream ecosystems and water quality [8]. Natural and synthetic estrogens, other pharmaceuticals and disease-causing bacteria are entering streams through the release of wastewater from sewage treatment plants and effluent from septic systems [9,10].

The present study is an attempt to characterize the trends in physico-chemical properties of water quality in Mudhol taluka, Karnataka, India and compare the results with WHO standards.

MATERIALS AND METHODS

Study area: Mudhol is a town previously known as "'Muduoolalu'" in the Bagalkot District in the Northern part of the South Indian state of Karnataka. It is about 60 km from the district headquarters of Bagalkot town on the left bank of the Ghataprabha River. It is famous for a breed of dog known as the Mudhol Hound. Mudhol State was ruled by the Ghorpade-Maratha royal family. The Principality of Mudhol ruled by the Ghorpade dynasty of the Marathas, was one of the 9-gun princely states of British India, under the summit of Niranjan. The state measured 368 square miles (508 km²) in area. According to the 1901 census, the population was 63,001, with the population of the town itself at 8,359 in that year. In 1901, the state enjoyed revenue estimated at £20,000. The state flag, called 'Bavuta', has a triangular tricolor of horizontal bands, in order from the top: white, black and green. All color bands came to the point in the fly. Birthplace of Vinay Koppad, founder of Youth For Unity and former co-founder of NaMo-Brigade. Youth For Unity is non government organization contribute towards Girl child

education, Rural Empowerment, Environment causes etc. Mudhol is located at 16.35°N 75.28°E.[1] It has an average elevation of 549 metres (1801 feet).

Sampling: Polythene bottle which were thoroughly washed thrice with the water to be analyzed. Samples of drinking water were collected in clean polyethylene bottles from different sources viz. tube well, bore well and hand pump in the monsoon ,pre and post monsoon from Mudhol taluka. The samples for physiochemical analysis were placed an ice box and transported to the laboratory for immediate analysis lie pH and EC were measured on-site by (using HACH sensION156 portable), respectively (APHA, 1998). TDS is calculated by the evaporation method, TH is determined by EDTA titration [11]. Chloride has been determined using spectrophotometer. The data have been compared with standard values which are given by Indian [12] and WHO [13] standards. Table 1 shows the seasonal variation of water quality of Mudhol taluka.

Material and Methods

Water samples from different sites were collected in polystyrene bottles. At each sampling location, composite surface water was collected and stored in clean polyethylene bottles that have been pre-washed with HNO3 and thoroughly rinsed with demonized water. Some physico-

chemical parameters like water pH, conductivity, Electrical conductivity ,total dissolved solid, Total hardness, were analyzed and recorded immediately after collection of the water samples. Analysis for the remaining physico-chemical parameters like calcium, magnesium and sulphate were carried out in the laboratory. The methods used for the estimation of the variables were standard methods of APHA [14] and Trivedy and Goel [15] .

Results and discussions

pH: The pH value of drinking water is an important index of acidity or alkalinity. Most of the waters are slightly alkaline due to presence of carbonates and bicarbonates. A number of minerals and organic matter interact with one another to give the resultant pH value of the sample. Among the ground water analyzed, maximum average pH values varied from 8.32 at S 31 and minimum average pH value 6.60 was observed at sample S 20 during pre monsoon. The pH value of different water samples show a mark fluctuation for the different sites. The range of pH value shows a variation from 7.16 at S4 to 8.21 at S 31 during monsoon season and 8.05 during postmonsoon,7.12 to 8.20 during monsoon and 7.02 S 20 to 8.01 at S 31 during post monsoon respectively. According to Fakayode [16], the pH of a water body is very important in determination of water quality since it affects other chemical reactions such as solubility and metal toxicity. The pHs of the water under study in all three seasons are within the WHO standard of 6.50-8.50.

Conductivity: Electrical conductivity is an important parameter for determining the water quality of domestic and agricultural purpose. The WHO permissible limit for EC in water is 600 mhos cm^{-1}, the germination of almost all the crops is affected and it may result in reduced yield [17]. Electrical conductivity is a measure of water capacity to conduct electrical current. It signifies the amount of total dissolved salts. In the present study EC values in the range of 2019 mhos cm^{-1} at S 11 to 2852 mhos cm^{-1} at S19 in pre monsoon,2126 mhos cm^{-1} at S10 to 2688 mhos cm^{-1} at S1, and 2175 mhos cm^{-1} at S44 to 2814 mhos cm^{-1} at S1 in post monsoon season respectively.

TDS: TDS is an important parameter which imparts a peculiar taste to water and reduce its potability. Desirable limit of TDS is 500mg/l (IS: 10500 standards) and maximum allowable limit is 1500 mg/l. The TDS of studied ground water samples varied between348.3 ppm atS1 to 1747ppm at S11 in premonsoon,108.6 ppm at S21 to 1877ppm at S1 in monsoon season and 869.5ppm at S44 to 1797.2ppm at S1 in post monsoon respectively. All the values obtained are

much higher than the limits. High TDS increase density of water, decrease solubility of gases like oxygen and ultimately make the water unsuitable for drinking [18]. High TDS level(>500mg/L) result in excessive scaling in water pipes, water heater, boilers, and household appliances [19].

Hardness: Hardness reflects the composite measure of polyvalent cations whereas calcium and magnesium is the primary constituent of hardness [20]. Public acceptability of the degree of hardness may vary considerably from one community to another. Hardness value above 200mg/L is generally unacceptable. There is no recent reliable data on possible adverse effects associated with hardness 200mg/L may cause scale deposition in distribution system as well as increase soap consumption. Hardness of studied ground water samples varied from 186.5 mg/L at S7 to 718.4 mg/L at S26 in pre-monsoon season,242.9 mg/L at S 21 to 799.9 mg/L in monsoon season and 261.9 mg/L at S 20 to 769.9 mg/L in post-monsoon respectively and most of the values are above the permissible limits of WHO.

Calcium: There is a significant variation in calcium content during the three seasons of investigation in all the sites which varied from 51.0 mg/L at S11 to 96.0 mg/L at S 19 mg/L in Pre-monsoon, 59.0 mg/L at S 21 to 88.0 mg/L at S24 in monsoon season and 51 mg/L at S11 to 80.0 mg/L at 19 in Post monsoon respectively. According to Bureau of Indian Standards [21], standard value for calcium is 75 mg/L and can be relaxed up to 200 mg/L. The higher value of calcium registered during the study period may be due to the influx of industrial waste and sewage to the river water . In estuarine water, the variation of concentration of calcium is quite significant due to land drainage, high rates of biological uptake, and precipitation and dissolution process characteristics of shallow system [22]. More than 50% of present water samples exceed the permissible limits.

Magnesium: As per BIS [21], prescribed standard limit for magnesium is 30-70 mg/L and hence the observed values were beyond the permissible limit. Calcium content of Mudhol taluka ranged from 48.0 mg/L at S13 to 86.o at S 9 in pre-monsoon, 55.0 mg/L at S 21 to 92.0 mg/L at S9 mg/L in monsoon season and 50.0 mg/L at S 17 to 98.0 mg/L at S 5 in post monsoon season respectively. As estuaries receive inputs from multiple sources of organic and inorganic matter such as materials exported from agricultural, urban development through drainage basin in to the river and intrusion of marine water from ocean during high tidal periods which contain multiple

ionic sources such as Ca^{+2}, Mg^{+2}, Cl^{-} etc may increase the magnesium content in the study sites [23].

Sulphate: The sources of sulphate in underground waters may be rocks, geological formation, and so on. Excess sulphate has a laxative effect, especially in combination with magnesium and/or sodium. Sulphates exist in nearly all natural waters, the concentrations varying according to the nature of the terrain through which they flow. They are often derived from the sulphides of heavy metals (iron, nickel, copper and lead). Iron sulphides are present in sedimentary rocks from which they can be oxidised to sulphate in humid climates; the latter may then leach into watercourses so that ground waters are often excessively high in sulphates[24]. As magnesium and sodium are present in many waters, their combination with sulphate will have an enhanced laxative effect of greater or lesser magnitude depending on concentration. The utility of water for domestic purposes will therefore be severely limited by high sulphate concentrations, hence the limit of 200 mg/dm^3 SO_4^{2-} [24]. The sulphate contents of all the water samples ranged from 140mg/L at S21 to 178mg/L in Pre-monsoon,141mg/L at S49 to 187mg/L at S9 in monsoon season season and 139mg/L to 166mg/L in post-monsoon season respectively. The sulphate contents of all the water samples fall below the MPL (200 mg/dm^3).

Conclusion

In this case study, different physico-chemical parameters were successfully applied and compared with the respective standards to monitor the water quality of Mudhol taluaka of Bagalkot district ,Karnataka India . Water analysis of pH, conductivity, TDS, hardness, calcium, magnesium and sulphate , are the most important parameters represent the pollution. status of the water. The pollutants are due to the release of effluents from several sources into the estuary, which causes significant changes in the quality of water and pose some deleterious effect to the mangrove ecosystem in a long run. The immediate need is to maintain existing sewage treatment plants so that effluent discharge has a minimum of suspended solids. As a result, it is essential that Mudhol taluka environment monitoring is urgently required.

Acknowledgements: Authors are grateful to the UGC New Delhi for providing financial support to carry out this study. We express our deep sense of gratitude to BLDE management Vijayapur, Principal and HOD Chemistry for their help and cooperation. We are grateful to the authorities permitting us to carry out the present study.

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S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.44	2968	1897.2	599.6	85	76	168
2	Sameerwadi public bore well	8.01	2755	1478.5	475.2	72	81	169
3	Belagali public bore well	7.52	2665	1309.2	419.6	75	79	169
4	Mugalkod public tap	7.36	2589	1206.6	482.5	79	79	169
5	Budni PM 1 public bore well	7.78	2654	1216.2	618.3	72	78	174
6	Budni PM 2 public bore well	7.61	2765	1332.1	495.2	79	78	171
7	Nagaral public bore well	7.81	2858	1252.3	398.6	79	79	169
8	Dhavaleshwar public bore well	7.46	2745	1208.6	455.9	77	79	156
9	Sanganatti public bore well	7.91	2869	1599.8	798.5	81	92	187
10	Vajjarmatti public bore well	7.71	2226	988.8	408.3	76	77	168
11	Lokapur public bore well	8.20	2229	995.6	420.4	66	65	166
12	Nandaganv public bore well	8.13	2868	1325.4	504.2	76	74	169
13	Akkimaradi public bore well	7.65	2525	1208.5	436.5	66	68	169
14	Sayadapur Public bore well	7.62	2435	1189.6	411.5	69	71	168
15	Mugalkod public bore well	7.62	2798	1318.5	469.5	79	77	177
16	Kullalli public tap	7.61	2745	1215.5	453.4	75	69	166
17	Mudhol public bore well budni road	7.79	2305	1122.5	438.6	66	62	161
18	Mudhol public bore well bilagi road	7.46	2758	1325.6	548.9	82	72	179
19	Mudhol public bore well near buss stand	7.57	2892	1481.7	809.9	89	76	188
20	Alagundi BK public bore well	7.12	2547	1152.6	461.7	69	68	162
21	Malapur public tap	8.02	2454	1118.6	428.9	63	62	168
22	Shirol public Bore well	8.12	2534	1107.8	409.2	68	72	170

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Table.1 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Pre Mansoon)

S No	**Area of Samples collected**	**pH**	EC	**TDS in ppm**	**Hardness in ppm**	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.02	2543	1547.1	559.5	70	65	141
2	Sameerwadi public bore well	7.89	2335	1125.2	413.3	60	65	150
3	Belagali public bore well	6.92	2254	1061.0	399.2	55	64	142
4	Mugalkod public tap	7.16	2289	1008.2	372.9	62	65	150
5	Budni PM 1 public bore well	7.21	2312	1002.0	368.2	61	67	156
6	Budni PM 2 public bore well	7.12	2485	1053.0	385.9	60	67	145
7	Nagaral public bore well	7.33	2588	1014.6	389.8	61	65	141
8	Dhavaleshwar public bore well	7.05	2443	1108.2	405.4	63	61	136
9	Sanganatti public bore well	7.55	2537	1408.6	758.3	71	80	164
10	Vajjarmatti public bore well	7.25	2004	869.3	369.2	56	58	141
11	Lokapur public bore well	8.02	1919	638.3	276.5	51	55	148
12	Nandaganv public bore well	7.33	2413	1184.6	437.6	62	60	150
13	Akkimaradi public bore well	7.45	2165	878.8	303.8	52	48	145
14	Sayadapur Public bore well	7.11	2198	965.4	332.6	60	55	143
15	Mugalkod public bore well	7.31	2445	1024.6	423.8	65	69	161
16	Kullalli public tap	7.18	2389	1085.8	399.3	62	54	151
17	Mudhol public bore well budni road	7.33	2025	1007.8	277.8	60	51	144
18	Mudhol public bore well bilagi road	7.22	2115	920.1	362.2	58	52	150
19	Mudhol public bore well near buss stand	7.47	2652	1381.5	769.9	86	70	171
20	Alagundi BK public bore well	6.48	2134	401.9	261.9	58	51	142
21	Malapur public tap	8.02	2174	1009.5	390.5	52	46	140

22	Shirol public Bore well	8.01	2256	1004.5	385.9	57	58	154
23	Shirol public tap water	7.80	2301	1016.4	395.9	52	54	152
24	Konnur public Bore well	7.43	2585	1087.4	418.4	72	69	170
25	Mantur public Bore well	7.59	2557	1006.4	389.4	56	60	141
26	Machaknur public Bore well	7.16	2684	1107.4	413.5	69	70	162
27	Timmapur public Bore well	7.29	2548	1005.3	387.2	66	61	145
28	Jeergal public Bore well	8.04	2454	989.3	385.6	66	61	152
29	Chichakandi public Bore well	7.66	2401	1008.8	375.4	61	52	141
30	Kasabajambagi public Bore well	7.15	2421	987.5	370.5	63	56	150
31	Malali public Bore well	7.75	2568	1105.4	389.7	65	54	153
32	Halagali public Bore well	7.39	2424	1007.3	385.3	60	51	145
33	Kataraki public Bore well	7.14	2489	1022.3	395.5	57	52	145
34	Muddapur public Bore well	7.72	2398	996.4	386.4	61	55	150
35	Bisanal public Bore well	8.02	2454	1007.2	384.7	64	66	161
36	Mahalingapur public Bore well	7.69	2415	1015.5	390.4	70	67	160
37	Madhabanvi public Bore well	7.59	2511	1084.3	416.6	63	62	152
38	Marapur public Bore well	7.82	2465	992.9	381.7	58	62	153
39	Hebbal public Bore well	7.37	2145	901.4	378.4	62	54	145
40	Soraganvi Bore well	7.07	2289	985.9	422.3	68	63	158
41	Alagur public Bore well	8.05	2101	988.5	418.7	60	54	141
42	Chikkalgundi public Bore well	7.77	2135	1037.4	459.7	62	67	161
43	Chikkur public Bore well	7.69	2391	1086.3	416.3	71	73	164
44	Bantanur public Bore well	8.01	2123	903.8	389.6	61	63	165
45	Bannurpublic Bore well	7.72	2566	1104.5	479.2	67	70	167

46	Rugi public Bore well	8.01	2167	1017.5	470.3	70	67	160
47	Jaliber public Bore well	7.78	2685	1102.3	479.5	75	72	161
48	Metagudda public Bore well	7.57	2402	1104.5	423.6	70	65	160
49	Dadanatti public Bore well	7.82	2275	1026.4	403.4	63	60	150
50	Baragi public Bore well	7.77	2362	1109.6	475.5	65	63	156

Table.2 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Mansoon)

23	Shirol public tap water	8.01	2589	11 26.5	417.5	69	71	168
24	Konnur public Bore well	7.72	2945	1408.6	802.6	87	88	184
25	Mantur public Bore well	7.99	2864	1325.3	732.8	70	71	168
26	Machaknur public Bore well	7.42	2894	1309.5	765.8	82	86	175
27	Timmapur public Bore well	7.51	2792	1238.4	705.3	77	79	170
28	Jeergal public Bore well	8.10	2698	1123.5	585.1	70	69	166
29	Chichakandi public Bore well	7.98	2698	1178.7	595.8	73	68	168
30	Kasabajambagi public Bore well	7.52	2723	1318.2	767.2	68	70	170
31	Malali public Bore well	8.31	2888	1472.5	785.9	72	73	172
32	Halagali public Bore well	7.68	2712	1377.5	702.5	68	69	163
33	Kataraki public Bore well	7.45	2898	1478.5	809.6	74	71	168
34	Muddapur public Bore well	8.12	2768	1266.5	715.9	71	70	168
35	Bisanal public Bore well	8.01	2712	1212.3	685.8	69	65	169
36	Mahalingapur public Bore well	7.57	2755	1243.2	695.8	71	75	171
37	Madhabanvi public Bore well	7.89	2889	1153.4	589.7	73	76	172
38	Marapur public Bore well	8.08	2724	1222.6	678.8	69	71	167
39	Hebbal public Bore well	7.77	2415	1185.5	525.6	62	63	168
40	Soraganvi Bore well	7.38	2536	1110.2	495.6	69	73	169
41	Alagur public Bore well	8.15	2401	1125.5	528.7	67	62	159
42	Chikkalgundi public Bore well	7.79	2335	1097.8	469.5	69	68	165
43	Chikkur public Bore well	7.78	2510	1136.7	543.8	73	74	169
44	Bantanur public Bore well	8.13	2340	1098.9	459.8	68	69	164
45	Bannurpublic Bore well	7.85	2661	1254.8	619.8	68	66	168
46	Rugi public Bore well	7.89	2445	1123.9	547.8	73	68	164

47	Jaliber public Bore well	7.79	2765	1344.8	715.9	71	68	162
48	Metagudda public Bore well	7.79	2512	1228.4	614.7	73	68	160
49	Dadanatti public Bore well	8.11	2414	1120.8	512.5	68	66	161
50	Baragi public Bore well	7.87	2522	1138.8	548.7	69	72	169

Table.3 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Post Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.12	2814	1797.2	576.8	78	73	166
2	Sameerwadi public bore well	7.41	2587	1289.6	447.1	60	71	153
3	Belagali public bore well	7.11	2489	1145.3	355.4	57	65	156
4	Mugalkod public tap	7.05	2404	1031.4	389.9	67	68	155
5	Budni PM 1 public bore well	7.11	2422	1049.3	565.4	63	98	160
6	Budni PM 2 public bore well	7.05	2581	1191.3	438.6	58	67	156
7	Nagaral public bore well	7.11	2689	1100.6	331.5	60	65	150
8	Dhavaleshwar public bore well	7.12	2509	1103.3	405.5	65	67	140
9	Sanganatti public bore well	7.32	2687	1401.5	706.6	70	78	160
10	Vajjarmatti public bore well	7.15	2009	1145.6	455.6	56	61	142
11	Lokapur public bore well	7.59	2045	938.4	459.8	52	53	141
12	Nandaganv public bore well	7.37	2671	1201.2	535.3	61	64	150
13	Akkimaradi public bore well	7.15	2315	1217.9	556.8	53	56	151
14	Sayadapur Public bore well	7.27	2249	1207.7	550.6	56	57	143
15	Mugalkod public bore well	7.32	2585	1088.4	426.7	68	65	156
16	Kullalli public tap	7.05	2520	1089.9	521.5	62	56	148
17	Mudhol public bore well budni road	7.32	2105	930.6	371.7	54	50	141
18	Mudhol public bore well bilagi road	7.02	2589	1146.8	603.7	70	56	151
19	Mudhol public bore well near buss stand	7.25	2788	1185.9	774.4	80	65	161
20	Alagundi BK public bore well	7.02	2358	1186.4	525.5	56	54	142
21	Malapur public tap	7.34	2287	1021.4	484.3	53	51	150
22	Shirol public Bore well	7.41	2335	1028.2	488.3	56	60	153

23	Shirol public tap water	7.57	2425	1051.8	471.8	54	61	153
24	Konnur public Bore well	7.33	2734	1326.2	673.8	70	72	170
25	Mantur public Bore well	7.55	2689	1035.5	588.5	58	61	145
26	Machaknur public Bore well	7.12	2735	1115.2	606.4	71	72	155
27	Timmapur public Bore well	7.28	2631	1038.8	544.8	65	68	152
28	Jeergal public Bore well	7.51	2504	1047.3	459.3	61	60	152
29	Chichakandi public Bore well	7.58	2507	1107.9	491.2	61	60	145
30	Kasabajambagi public Bore well	7.12	2536	1046.8	422.8	53	60	150
31	Malali public Bore well	8.01	2701	1178.8	548.4	56	60	153
32	Halagali public Bore well	7.26	2514	1083.4	441.8	55	61	152
33	Kataraki public Bore well	7.11	2716	1087.6	662.4	60	62	151
34	Muddapur public Bore well	7.72	2485	1015.3	395.3	59	61	151
35	Bisanal public Bore well	7.67	2511	1025.5	451.7	51	60	155
36	Mahalingapur public Bore well	7.19	2586	1025.3	531.6	62	65	160
37	Madhabanvi public Bore well	7.59	2604	1084.5	579.2	63	67	155
38	Marapur public Bore well	7.72	2510	1013.7	502.4	57	63	153
39	Hebbal public Bore well	7.32	2211	966.9	378.4	56	65	154
40	Soraganvi Bore well	7.10	2374	1022.8	364.2	55	61	151
41	Alagur public Bore well	7.78	2205	1015.8	361.8	54	51	140
42	Chikkalgundi public Bore well	7.55	2184	959.5	345.6	52	60	145
43	Chikkur public Bore well	7.54	2322	1001.8	509.7	60	62	150
44	Bantanur public Bore well	7.72	2175	869.5	311.4	52	53	145
45	Bannurpublic Bore well	7.57	2478	1087.1	468.4	52	54	151
46	Rugi public Bore well	7.61	2279	950.7	375.7	62	54	141

47	Jaliber public Bore well	7.51	2584	1021.7	472.7	68	60	146
48	Metagudda public Bore well	7.47	2304	1021.5	459.8	62	51	140
49	Dadanatti public Bore well	8.01	2292	1066.8	410.4	61	59	139
50	Baragi public Bore well	7.55	2389	1065.9	482.8	68	59	155

ASSESSMENT OF SEASONAL VARIATIONS IN WATER QUALITY OF MUDHOL TALUKA IN BAGALKOT DISTRICT, KARNATAKA INDIA .

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Abstract: Assessment of seasonal changes in surface water quality is an important aspect for evaluating temporal variations of water pollution due to natural or anthropogenic inputs of point and non-point sources. In this study, surface water quality data for 7 physical and chemical parameters collected from 50 monitoring stations in a water of Mudhol taluka of Bagalkot district, Karnataka were analyzed. The principal component analysis technique was employed to evaluate the seasonal variations of water quality parameters, while the principal factor analysis technique was used to extract the parameters that are most important in assessing seasonal variations of water quality. Analysis shows that a parameter that is most important in contributing to water quality variation for one season may not be important for another season except for DOC and electrical conductance, which were always the most important parameters in contributing to water quality variations for all four seasons

Introduction

Water is the most vital resources for all kinds of life on this planet. Water is one of the nature's most important gifts to mankind. It is essential and most precious commodity for life. Rivers are vital and vulnerable freshwater systems and are essential for the sustenance of all life. Pollution of surface water with toxic chemicals and eutro-phication of rivers and lakes with excess nutrients are of great environmental concern worldwide. Agricultural, Indus-trial, and urban activities are considered as being major sources of chemicals and nutrients to aquatic ecosystems, while atmospheric deposition could be an important source to certain constituents such as mercury and nitrogen. The concentrations of toxic chemicals and biologically available nutrients in excess can lead to diverse problems such as toxic algal blooms, loss of oxygen, fish kills, loss of biodiversity, and loss of aquatic plant beds and coal reefs [1]. Nutrient enrichment seriously degrades aquatic ecosystems and impairs the use of water for drinking, industry, agriculture, and recreation and for other purposes. The modern civilization, urbanization and prolonged discharge of industrial effluents, domestic sewage and solid waste dump cause the water to became polluted. Wild and domestic animals using same drinking water can also contaminate the water through direct defection and urination [2]. The modern civilization, urbanization and prolonged discharge of industrial effluents, domestic sewage and solid waste dump cause the water to became polluted. Wild and domestic animals using same

drinking water can also contaminate the water through direct defection and urination [3]. Rivers are considered as vital and vulnerable freshwater ecosystems that are important for the sustenance of all life. Untreated discharge of pollutants to a water resource system from domestic sources, storm water discharges, industrial wastewaters, agricultural runoff and the other sources, all can have short term and long term significant effects on the quality of a river system[4]. The physico-chemical parameters useful for water quality assessment are determined by the presence of both organic and inorganic compounds that are either suspended or dissolved in water. At the same time, water quality characteristics of aquatic environment arise from a multitude of physical, chemical and biological interactions [5]. While some of these compounds are toxic to the ecosystem, some are providing nutrients to aquatic organisms and others are responsible for the aesthetics of the water body[6]. Human activities are a major factor determining the quality of the surface and ground water through atmospheric pollution, effluent discharges, use of agricultural chemicals, eroded soils and land use [7]. These land use changes increase the amount of impervious surface resulting in storm runoff events that negatively affect stream ecosystems and water quality [8]. Natural and synthetic estrogens, other pharmaceuticals and disease-causing bacteria are entering streams through the release of wastewater from sewage treatment plants and effluent from septic systems [9,10].

The present study is an attempt to characterize the trends in physico-chemical properties of water quality in Mudhol taluka, Karnataka, India and compare the results with WHO standards.

MATERIALS AND METHODS

Study area: Mudhol is a town previously known as "'Muduoolalu'" in the Bagalkot District in the Northern part of the South Indian state of Karnataka. It is about 60 km from the district headquarters of Bagalkot town on the left bank of the Ghataprabha River. It is famous for a breed of dog known as the Mudhol Hound. Mudhol State was ruled by the Ghorpade-Maratha royal family. The Principality of Mudhol ruled by the Ghorpade dynasty of the Marathas, was one of the 9-gun princely states of British India, under the summit of Niranjan. The state measured 368 square miles (508 km²) in area. According to the 1901 census, the population was 63,001, with the population of the town itself at 8,359 in that year. In 1901, the state enjoyed revenue estimated at £20,000. The state flag, called 'Bavuta', has a triangular tricolor of horizontal bands, in order from the top: white, black and green. All color bands came to the point in the fly. Birthplace of Vinay Koppad, founder of Youth For Unity and former co-founder of NaMo-Brigade. Youth For Unity is non government organization contribute towards Girl child

education, Rural Empowerment, Environment causes etc. Mudhol is located at 16.35°N 75.28°E.[1] It has an average elevation of 549 metres (1801 feet).

Sampling: Polythene bottle which were thoroughly washed thrice with the water to be analyzed. Samples of drinking water were collected in clean polyethylene bottles from different sources viz. tube well, bore well and hand pump in the monsoon ,pre and post monsoon from Mudhol taluka. The samples for physiochemical analysis were placed an ice box and transported to the laboratory for immediate analysis lie pH and EC were measured on-site by (using HACH sensION156 portable), respectively (APHA, 1998). TDS is calculated by the evaporation method, TH is determined by EDTA titration [11]. Chloride has been determined using spectrophotometer. The data have been compared with standard values which are given by Indian [12] and WHO [13] standards. Table 1 shows the seasonal variation of water quality of Mudhol taluka.

Material and Methods

Water samples from different sites were collected in polystyrene bottles. At each sampling location, composite surface water was collected and stored in clean polyethylene bottles that have been pre-washed with HNO3 and thoroughly rinsed with demonized water. Some physico-

chemical parameters like water pH, conductivity, Electrical conductivity ,total dissolved solid, Total hardness, were analyzed and recorded immediately after collection of the water samples. Analysis for the remaining physico-chemical parameters like calcium, magnesium and sulphate were carried out in the laboratory. The methods used for the estimation of the variables were standard methods of APHA [14] and Trivedy and Goel [15] .

Results and discussions

pH: The pH value of drinking water is an important index of acidity or alkalinity. Most of the waters are slightly alkaline due to presence of carbonates and bicarbonates. A number of minerals and organic matter interact with one another to give the resultant pH value of the sample. Among the ground water analyzed, maximum average pH values varied from 8.32 at S 31 and minimum average pH value 6.60 was observed at sample S 20 during pre monsoon. The pH value of different water samples show a mark fluctuation for the different sites. The range of pH value shows a variation from 7.16 at S4 to 8.21 at S 31 during monsoon season and 8.05 during postmonsoon,7.12 to 8.20 during monsoon and 7.02 S 20 to 8.01 at S 31 during post monsoon respectively. According to Fakayode [16], the pH of a water body is very important in determination of water quality since it affects other chemical reactions such as solubility and metal toxicity. The pHs of the water under study in all three seasons are within the WHO standard of 6.50-8.50.

Conductivity: Electrical conductivity is an important parameter for determining the water quality of domestic and agricultural purpose. The WHO permissible limit for EC in water is 600 mhos cm^{-1}, the germination of almost all the crops is affected and it may result in reduced yield [17]. Electrical conductivity is a measure of water capacity to conduct electrical current. It signifies the amount of total dissolved salts. In the present study EC values in the range of 2019 mhos cm^{-1} at S 11 to 2852 mhos cm^{-1} at S19 in pre monsoon,2126 mhos cm^{-1} at S10 to 2688 mhos cm^{-1} at S1, and 2175 mhos cm^{-1} at S44 to 2814 mhos cm^{-1} at S1 in post monsoon season respectively.

TDS: TDS is an important parameter which imparts a peculiar taste to water and reduce its potability. Desirable limit of TDS is 500mg/l (IS: 10500 standards) and maximum allowable limit is 1500 mg/l. The TDS of studied ground water samples varied between348.3 ppm atS1 to 1747ppm at S11 in premonsoon,108.6 ppm at S21 to 1877ppm at S1 in monsoon season and 869.5ppm at S44 to 1797.2ppm at S1 in post monsoon respectively. All the values obtained are

much higher than the limits. High TDS increase density of water, decrease solubility of gases like oxygen and ultimately make the water unsuitable for drinking [18]. High TDS level(>500mg/L) result in excessive scaling in water pipes, water heater, boilers, and household appliances [19].

Hardness: Hardness reflects the composite measure of polyvalent cations whereas calcium and magnesium is the primary constituent of hardness [20]. Public acceptability of the degree of hardness may vary considerably from one community to another. Hardness value above 200mg/L is generally unacceptable. There is no recent reliable data on possible adverse effects associated with hardness 200mg/L may cause scale deposition in distribution system as well as increase soap consumption. Hardness of studied ground water samples varied from 186.5 mg/L at S7 to 718.4 mg/L at S26 in pre-monsoon season,242.9 mg/L at S 21 to 799.9 mg/L in monsoon season and 261.9 mg/L at S 20 to 769.9 mg/L in post-monsoon respectively and most of the values are above the permissible limits of WHO.

Calcium: There is a significant variation in calcium content during the three seasons of investigation in all the sites which varied from 51.0 mg/L at S11 to 96.0 mg/L at S 19 mg/L in Pre-monsoon, 59.0 mg/L at S 21 to 88.0 mg/L at S24 in monsoon season and 51 mg/L at S11 to 80.0 mg/L at 19 in Post monsoon respectively. According to Bureau of Indian Standards [21], standard value for calcium is 75 mg/L and can be relaxed up to 200 mg/L. The higher value of calcium registered during the study period may be due to the influx of industrial waste and sewage to the river water . In estuarine water, the variation of concentration of calcium is quite significant due to land drainage, high rates of biological uptake, and precipitation and dissolution process characteristics of shallow system [22]. More than 50% of present water samples exceed the permissible limits.

Magnesium: As per BIS [21], prescribed standard limit for magnesium is 30-70 mg/L and hence the observed values were beyond the permissible limit. Calcium content of Mudhol taluka ranged from 48.0 mg/L at S13 to 86.o at S 9 in pre-monsoon, 55.0 mg/L at S 21 to 92.0 mg/L at S9 mg/L in monsoon season and 50.0 mg/L at S 17 to 98.0 mg/L at S 5 in post monsoon season respectively. As estuaries receive inputs from multiple sources of organic and inorganic matter such as materials exported from agricultural, urban development through drainage basin in to the river and intrusion of marine water from ocean during high tidal periods which contain multiple

ionic sources such as Ca^{+2}, Mg^{+2}, Cl^- etc may increase the magnesium content in the study sites [23].

Sulphate: The sources of sulphate in underground waters may be rocks, geological formation, and so on. Excess sulphate has a laxative effect, especially in combination with magnesium and/or sodium. Sulphates exist in nearly all natural waters, the concentrations varying according to the nature of the terrain through which they flow. They are often derived from the sulphides of heavy metals (iron, nickel, copper and lead). Iron sulphides are present in sedimentary rocks from which they can be oxidised to sulphate in humid climates; the latter may then leach into watercourses so that ground waters are often excessively high in sulphates[24]. As magnesium and sodium are present in many waters, their combination with sulphate will have an enhanced laxative effect of greater or lesser magnitude depending on concentration. The utility of water for domestic purposes will therefore be severely limited by high sulphate concentrations, hence the limit of 200 mg/dm^3 SO_4^{2-} [24]. The sulphate contents of all the water samples ranged from 140mg/L at S21 to 178mg/L in Pre-monsoon,141mg/L at S49 to 187mg/L at S9 in monsoon season season and 139mg/L to 166mg/L in post-monsoon season respectively. The sulphate contents of all the water samples fall below the MPL (200 mg/dm^3).

Conclusion

In this case study, different physico-chemical parameters were successfully applied and compared with the respective standards to monitor the water quality of Mudhol taluaka of Bagalkot district ,Karnataka India . Water analysis of pH, conductivity, TDS, hardness, calcium, magnesium and sulphate , are the most important parameters represent the pollution. status of the water. The pollutants are due to the release of effluents from several sources into the estuary, which causes significant changes in the quality of water and pose some deleterious effect to the mangrove ecosystem in a long run. The immediate need is to maintain existing sewage treatment plants so that effluent discharge has a minimum of suspended solids. As a result, it is essential that Mudhol taluka environment monitoring is urgently required.

Acknowledgements: Authors are grateful to the UGC New Delhi for providing financial support to carry out this study. We express our deep sense of gratitude to BLDE management Vijayapur, Principal and HOD Chemistry for their help and cooperation. We are grateful to the authorities permitting us to carry out the present study.

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Table.1 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Pre Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.02	2543	1547.1	559.5	70	65	141
2	Sameerwadi public bore well	7.89	2335	1125.2	413.3	60	65	150
3	Belagali public bore well	6.92	2254	1061.0	399.2	55	64	142
4	Mugalkod public tap	7.16	2289	1008.2	372.9	62	65	150
5	Budni PM 1 public bore well	7.21	2312	1002.0	368.2	61	67	156
6	Budni PM 2 public bore well	7.12	2485	1053.0	385.9	60	67	145
7	Nagaral public bore well	7.33	2588	1014.6	389.8	61	65	141
8	Dhavaleshwar public bore well	7.05	2443	1108.2	405.4	63	61	136
9	Sanganatti public bore well	7.55	2537	1408.6	758.3	71	80	164
10	Vajjarmatti public bore well	7.25	2004	869.3	369.2	56	58	141
11	Lokapur public bore well	8.02	1919	638.3	276.5	51	55	148
12	Nandaganv public bore well	7.33	2413	1184.6	437.6	62	60	150
13	Akkimaradi public bore well	7.45	2165	878.8	303.8	52	48	145
14	Sayadapur Public bore well	7.11	2198	965.4	332.6	60	55	143
15	Mugalkod public bore well	7.31	2445	1024.6	423.8	65	69	161
16	Kullalli public tap	7.18	2389	1085.8	399.3	62	54	151
17	Mudhol public bore well budni road	7.33	2025	1007.8	277.8	60	51	144
18	Mudhol public bore well bilagi road	7.22	2115	920.1	362.2	58	52	150
19	Mudhol public bore well near buss stand	7.47	2652	1381.5	769.9	86	70	171
20	Alagundi BK public bore well	6.48	2134	401.9	261.9	58	51	142
21	Malapur public tap	8.02	2174	1009.5	390.5	52	46	140

22	Shirol public Bore well	8.01	2256	1004.5	385.9	57	58	154
23	Shirol public tap water	7.80	2301	1016.4	395.9	52	54	152
24	Konnur public Bore well	7.43	2585	1087.4	418.4	72	69	170
25	Mantur public Bore well	7.59	2557	1006.4	389.4	56	60	141
26	Machaknur public Bore well	7.16	2684	1107.4	413.5	69	70	162
27	Timmapur public Bore well	7.29	2548	1005.3	387.2	66	61	145
28	Jeergal public Bore well	8.04	2454	989.3	385.6	66	61	152
29	Chichakandi public Bore well	7.66	2401	1008.8	375.4	61	52	141
30	Kasabajambagi public Bore well	7.15	2421	987.5	370.5	63	56	150
31	Malali public Bore well	7.75	2568	1105.4	389.7	65	54	153
32	Halagali public Bore well	7.39	2424	1007.3	385.3	60	51	145
33	Kataraki public Bore well	7.14	2489	1022.3	395.5	57	52	145
34	Muddapur public Bore well	7.72	2398	996.4	386.4	61	55	150
35	Bisanal public Bore well	8.02	2454	1007.2	384.7	64	66	161
36	Mahalingapur public Bore well	7.69	2415	1015.5	390.4	70	67	160
37	Madhabanvi public Bore well	7.59	2511	1084.3	416.6	63	62	152
38	Marapur public Bore well	7.82	2465	992.9	381.7	58	62	153
39	Hebbal public Bore well	7.37	2145	901.4	378.4	62	54	145
40	Soraganvi Bore well	7.07	2289	985.9	422.3	68	63	158
41	Alagur public Bore well	8.05	2101	988.5	418.7	60	54	141
42	Chikkalgundi public Bore well	7.77	2135	1037.4	459.7	62	67	161
43	Chikkur public Bore well	7.69	2391	1086.3	416.3	71	73	164
44	Bantanur public Bore well	8.01	2123	903.8	389.6	61	63	165
45	Bannurpublic Bore well	7.72	2566	1104.5	479.2	67	70	167

46	Rugi public Bore well	8.01	2167	1017.5	470.3	70	67	160
47	Jaliber public Bore well	7.78	2685	1102.3	479.5	75	72	161
48	Metagudda public Bore well	7.57	2402	1104.5	423.6	70	65	160
49	Dadanatti public Bore well	7.82	2275	1026.4	403.4	63	60	150
50	Baragi public Bore well	7.77	2362	1109.6	475.5	65	63	156

Table.2 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.44	2968	1897.2	599.6	85	76	168
2	Sameerwadi public bore well	8.01	2755	1478.5	475.2	72	81	169
3	Belagali public bore well	7.52	2665	1309.2	419.6	75	79	169
4	Mugalkod public tap	7.36	2589	1206.6	482.5	79	79	169
5	Budni PM 1 public bore well	7.78	2654	1216.2	618.3	72	78	174
6	Budni PM 2 public bore well	7.61	2765	1332.1	495.2	79	78	171
7	Nagaral public bore well	7.81	2858	1252.3	398.6	79	79	169
8	Dhavaleshwar public bore well	7.46	2745	1208.6	455.9	77	79	156
9	Sanganatti public bore well	7.91	2869	1599.8	798.5	81	92	187
10	Vajjarmatti public bore well	7.71	2226	988.8	408.3	76	77	168
11	Lokapur public bore well	8.20	2229	995.6	420.4	66	65	166
12	Nandaganv public bore well	8.13	2868	1325.4	504.2	76	74	169
13	Akkimaradi public bore well	7.65	2525	1208.5	436.5	66	68	169
14	Sayadapur Public bore well	7.62	2435	1189.6	411.5	69	71	168
15	Mugalkod public bore well	7.62	2798	1318.5	469.5	79	77	177
16	Kullalli public tap	7.61	2745	1215.5	453.4	75	69	166
17	Mudhol public bore well budni road	7.79	2305	1122.5	438.6	66	62	161
18	Mudhol public bore well bilagi road	7.46	2758	1325.6	548.9	82	72	179
19	Mudhol public bore well near buss stand	7.57	2892	1481.7	809.9	89	76	188
20	Alagundi BK public bore well	7.12	2547	1152.6	461.7	69	68	162
21	Malapur public tap	8.02	2454	1118.6	428.9	63	62	168
22	Shirol public Bore well	8.12	2534	1107.8	409.2	68	72	170

23	Shirol public tap water	8.01	2589	11 26.5	417.5	69	71	168
24	Konnur public Bore well	7.72	2945	1408.6	802.6	87	88	184
25	Mantur public Bore well	7.99	2864	1325.3	732.8	70	71	168
26	Machaknur public Bore well	7.42	2894	1309.5	765.8	82	86	175
27	Timmapur public Bore well	7.51	2792	1238.4	705.3	77	79	170
28	Jeergal public Bore well	8.10	2698	1123.5	585.1	70	69	166
29	Chichakandi public Bore well	7.98	2698	1178.7	595.8	73	68	168
30	Kasabajambagi public Bore well	7.52	2723	1318.2	767.2	68	70	170
31	Malali public Bore well	8.31	2888	1472.5	785.9	72	73	172
32	Halagali public Bore well	7.68	2712	1377.5	702.5	68	69	163
33	Kataraki public Bore well	7.45	2898	1478.5	809.6	74	71	168
34	Muddapur public Bore well	8.12	2768	1266.5	715.9	71	70	168
35	Bisanal public Bore well	8.01	2712	1212.3	685.8	69	65	169
36	Mahalingapur public Bore well	7.57	2755	1243.2	695.8	71	75	171
37	Madhabanvi public Bore well	7.89	2889	1153.4	589.7	73	76	172
38	Marapur public Bore well	8.08	2724	1222.6	678.8	69	71	167
39	Hebbal public Bore well	7.77	2415	1185.5	525.6	62	63	168
40	Soraganvi Bore well	7.38	2536	1110.2	495.6	69	73	169
41	Alagur public Bore well	8.15	2401	1125.5	528.7	67	62	159
42	Chikkalgundi public Bore well	7.79	2335	1097.8	469.5	69	68	165
43	Chikkur public Bore well	7.78	2510	1136.7	543.8	73	74	169
44	Bantanur public Bore well	8.13	2340	1098.9	459.8	68	69	164
45	Bannurpublic Bore well	7.85	2661	1254.8	619.8	68	66	168
46	Rugi public Bore well	7.89	2445	1123.9	547.8	73	68	164

47	Jaliber public Bore well	7.79	2765	1344.8	715.9	71	68	162
48	Metagudda public Bore well	7.79	2512	1228.4	614.7	73	68	160
49	Dadanatti public Bore well	8.11	2414	1120.8	512.5	68	66	161
50	Baragi public Bore well	7.87	2522	1138.8	548.7	69	72	169

Table.3 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Post Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO$_4$
1	Kesargoppa public bore well	7.12	2814	1797.2	576.8	78	73	166
2	Sameerwadi public bore well	7.41	2587	1289.6	447.1	60	71	153
3	Belagali public bore well	7.11	2489	1145.3	355.4	57	65	156
4	Mugalkod public tap	7.05	2404	1031.4	389.9	67	68	155
5	Budni PM 1 public bore well	7.11	2422	1049.3	565.4	63	98	160
6	Budni PM 2 public bore well	7.05	2581	1191.3	438.6	58	67	156
7	Nagaral public bore well	7.11	2689	1100.6	331.5	60	65	150
8	Dhavaleshwar public bore well	7.12	2509	1103.3	405.5	65	67	140
9	Sanganatti public bore well	7.32	2687	1401.5	706.6	70	78	160
10	Vajjarmatti public bore well	7.15	2009	1145.6	455.6	56	61	142
11	Lokapur public bore well	7.59	2045	938.4	459.8	52	53	141
12	Nandaganv public bore well	7.37	2671	1201.2	535.3	61	64	150
13	Akkimaradi public bore well	7.15	2315	1217.9	556.8	53	56	151
14	Sayadapur Public bore well	7.27	2249	1207.7	550.6	56	57	143
15	Mugalkod public bore well	7.32	2585	1088.4	426.7	68	65	156
16	Kullalli public tap	7.05	2520	1089.9	521.5	62	56	148
17	Mudhol public bore well budni road	7.32	2105	930.6	371.7	54	50	141
18	Mudhol public bore well bilagi road	7.02	2589	1146.8	603.7	70	56	151
19	Mudhol public bore well near buss stand	7.25	2788	1185.9	774.4	80	65	161
20	Alagundi BK public bore well	7.02	2358	1186.4	525.5	56	54	142
21	Malapur public tap	7.34	2287	1021.4	484.3	53	51	150
22	Shirol public Bore well	7.41	2335	1028.2	488.3	56	60	153

23	Shirol public tap water	7.57	2425	1051.8	471.8	54	61	153
24	Konnur public Bore well	7.33	2734	1326.2	673.8	70	72	170
25	Mantur public Bore well	7.55	2689	1035.5	588.5	58	61	145
26	Machaknur public Bore well	7.12	2735	1115.2	606.4	71	72	155
27	Timmapur public Bore well	7.28	2631	1038.8	544.8	65	68	152
28	Jeergal public Bore well	7.51	2504	1047.3	459.3	61	60	152
29	Chichakandi public Bore well	7.58	2507	1107.9	491.2	61	60	145
30	Kasabajambagi public Bore well	7.12	2536	1046.8	422.8	53	60	150
31	Malali public Bore well	8.01	2701	1178.8	548.4	56	60	153
32	Halagali public Bore well	7.26	2514	1083.4	441.8	55	61	152
33	Kataraki public Bore well	7.11	2716	1087.6	662.4	60	62	151
34	Muddapur public Bore well	7.72	2485	1015.3	395.3	59	61	151
35	Bisanal public Bore well	7.67	2511	1025.5	451.7	51	60	155
36	Mahalingapur public Bore well	7.19	2586	1025.3	531.6	62	65	160
37	Madhabanvi public Bore well	7.59	2604	1084.5	579.2	63	67	155
38	Marapur public Bore well	7.72	2510	1013.7	502.4	57	63	153
39	Hebbal public Bore well	7.32	2211	966.9	378.4	56	65	154
40	Soraganvi Bore well	7.10	2374	1022.8	364.2	55	61	151
41	Alagur public Bore well	7.78	2205	1015.8	361.8	54	51	140
42	Chikkalgundi public Bore well	7.55	2184	959.5	345.6	52	60	145
43	Chikkur public Bore well	7.54	2322	1001.8	509.7	60	62	150
44	Bantanur public Bore well	7.72	2175	869.5	311.4	52	53	145
45	Bannurpublic Bore well	7.57	2478	1087.1	468.4	52	54	151
46	Rugi public Bore well	7.61	2279	950.7	375.7	62	54	141

47	Jaliber public Bore well	7.51	2584	1021.7	472.7	68	60	146
48	Metagudda public Bore well	7.47	2304	1021.5	459.8	62	51	140
49	Dadanatti public Bore well	8.01	2292	1066.8	410.4	61	59	139
50	Baragi public Bore well	7.55	2389	1065.9	482.8	68	59	155

ASSESSMENT OF SEASONAL VARIATIONS IN WATER QUALITY OF MUDHOL TALUKA IN BAGALKOT DISTRICT, KARNATAKA INDIA .

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Abstract: Assessment of seasonal changes in surface water quality is an important aspect for evaluating temporal variations of water pollution due to natural or anthropogenic inputs of point and non-point sources. In this study, surface water quality data for 7 physical and chemical parameters collected from 50 monitoring stations in a water of Mudhol taluka of Bagalkot district, Karnataka were analyzed. The principal component analysis technique was employed to evaluate the seasonal variations of water quality parameters, while the principal factor analysis technique was used to extract the parameters that are most important in assessing seasonal variations of water quality. Analysis shows that a parameter that is most important in contributing to water quality variation for one season may not be important for another season except for DOC and electrical conductance, which were always the most important parameters in contributing to water quality variations for all four seasons

Introduction

Water is the most vital resources for all kinds of life on this planet. Water is one of the nature’s most important gifts to mankind. It is essential and most precious commodity for life. Rivers are vital and vulnerable freshwater systems and are essential for the sustenance of all life. Pollution of surface water with toxic chemicals and eutro-phication of rivers and lakes with excess nutrients are of great environmental concern worldwide. Agricultural, Indus-trial, and urban activities are considered as being major sources of chemicals and nutrients to aquatic ecosystems, while atmospheric deposition could be an important source to certain constituents such as mercury and nitrogen. The concentrations of toxic chemicals and biologically available nutrients in excess can lead to diverse problems such as toxic algal blooms, loss of oxygen, fish kills, loss of biodiversity, and loss of aquatic plant beds and coal reefs [1]. Nutrient enrichment seriously degrades aquatic ecosystems and impairs the use of water for drinking, industry, agriculture, and recreation and for other purposes. The modern civilization, urbanization and prolonged discharge of industrial effluents, domestic sewage and solid waste dump cause the water to became polluted. Wild and domestic animals using same drinking water can also contaminate the water through direct defection and urination [2]. The modern civilization, urbanization and prolonged discharge of industrial effluents, domestic sewage and solid waste dump cause the water to became polluted. Wild and domestic animals using same

drinking water can also contaminate the water through direct defection and urination [3]. Rivers are considered as vital and vulnerable freshwater ecosystems that are important for the sustenance of all life. Untreated discharge of pollutants to a water resource system from domestic sources, storm water discharges, industrial wastewaters, agricultural runoff and the other sources, all can have short term and long term significant effects on the quality of a river system[4]. The physico-chemical parameters useful for water quality assessment are determined by the presence of both organic and inorganic compounds that are either suspended or dissolved in water. At the same time, water quality characteristics of aquatic environment arise from a multitude of physical, chemical and biological interactions [5]. While some of these compounds are toxic to the ecosystem, some are providing nutrients to aquatic organisms and others are responsible for the aesthetics of the water body[6]. Human activities are a major factor determining the quality of the surface and ground water through atmospheric pollution, effluent discharges, use of agricultural chemicals, eroded soils and land use [7]. These land use changes increase the amount of impervious surface resulting in storm runoff events that negatively affect stream ecosystems and water quality [8]. Natural and synthetic estrogens, other pharmaceuticals and disease-causing bacteria are entering streams through the release of wastewater from sewage treatment plants and effluent from septic systems [9,10].

The present study is an attempt to characterize the trends in physico-chemical properties of water quality in Mudhol taluka, Karnataka, India and compare the results with WHO standards.

MATERIALS AND METHODS

Study area: Mudhol is a town previously known as "'Muduoolalu'" in the Bagalkot District in the Northern part of the South Indian state of Karnataka. It is about 60 km from the district headquarters of Bagalkot town on the left bank of the Ghataprabha River. It is famous for a breed of dog known as the Mudhol Hound. Mudhol State was ruled by the Ghorpade-Maratha royal family. The Principality of Mudhol ruled by the Ghorpade dynasty of the Marathas, was one of the 9-gun princely states of British India, under the summit of Niranjan. The state measured 368 square miles (508 km²) in area. According to the 1901 census, the population was 63,001, with the population of the town itself at 8,359 in that year. In 1901, the state enjoyed revenue estimated at £20,000. The state flag, called 'Bavuta', has a triangular tricolor of horizontal bands, in order from the top: white, black and green. All color bands came to the point in the fly. Birthplace of Vinay Koppad, founder of Youth For Unity and former co-founder of NaMo-Brigade. Youth For Unity is non government organization contribute towards Girl child

education, Rural Empowerment, Environment causes etc. Mudhol is located at 16.35°N 75.28°E.[1] It has an average elevation of 549 metres (1801 feet).

Sampling: Polythene bottle which were thoroughly washed thrice with the water to be analyzed. Samples of drinking water were collected in clean polyethylene bottles from different sources viz. tube well, bore well and hand pump in the monsoon ,pre and post monsoon from Mudhol taluka. The samples for physiochemical analysis were placed an ice box and transported to the laboratory for immediate analysis lie pH and EC were measured on-site by (using HACH sensION156 portable), respectively (APHA, 1998). TDS is calculated by the evaporation method, TH is determined by EDTA titration [11]. Chloride has been determined using spectrophotometer. The data have been compared with standard values which are given by Indian [12] and WHO [13] standards. Table 1 shows the seasonal variation of water quality of Mudhol taluka.

Material and Methods

Water samples from different sites were collected in polystyrene bottles. At each sampling location, composite surface water was collected and stored in clean polyethylene bottles that have been pre-washed with HNO3 and thoroughly rinsed with demonized water. Some physico-

chemical parameters like water pH, conductivity, Electrical conductivity ,total dissolved solid, Total hardness, were analyzed and recorded immediately after collection of the water samples. Analysis for the remaining physico-chemical parameters like calcium, magnesium and sulphate were carried out in the laboratory. The methods used for the estimation of the variables were standard methods of APHA [14] and Trivedy and Goel [15] .

Results and discussions

pH: The pH value of drinking water is an important index of acidity or alkalinity. Most of the waters are slightly alkaline due to presence of carbonates and bicarbonates. A number of minerals and organic matter interact with one another to give the resultant pH value of the sample. Among the ground water analyzed, maximum average pH values varied from 8.32 at S 31 and minimum average pH value 6.60 was observed at sample S 20 during pre monsoon. The pH value of different water samples show a mark fluctuation for the different sites. The range of pH value shows a variation from 7.16 at S4 to 8.21 at S 31 during monsoon season and 8.05 during postmonsoon,7.12 to 8.20 during monsoon and 7.02 S 20 to 8.01 at S 31 during post monsoon respectively. According to Fakayode [16], the pH of a water body is very important in determination of water quality since it affects other chemical reactions such as solubility and metal toxicity. The pHs of the water under study in all three seasons are within the WHO standard of 6.50-8.50.

Conductivity: Electrical conductivity is an important parameter for determining the water quality of domestic and agricultural purpose. The WHO permissible limit for EC in water is 600 mhos cm^{-1}, the germination of almost all the crops is affected and it may result in reduced yield [17]. Electrical conductivity is a measure of water capacity to conduct electrical current. It signifies the amount of total dissolved salts. In the present study EC values in the range of 2019 mhos cm^{-1} at S 11 to 2852 mhos cm^{-1} at S19 in pre monsoon,2126 mhos cm^{-1} at S10 to 2688 mhos cm^{-1} at S1, and 2175 mhos cm^{-1} at S44 to 2814 mhos cm^{-1} at S1 in post monsoon season respectively.

TDS: TDS is an important parameter which imparts a peculiar taste to water and reduce its potability. Desirable limit of TDS is 500mg/l (IS: 10500 standards) and maximum allowable limit is 1500 mg/l. The TDS of studied ground water samples varied between348.3 ppm atS1 to 1747ppm at S11 in premonsoon,108.6 ppm at S21 to 1877ppm at S1 in monsoon season and 869.5ppm at S44 to 1797.2ppm at S1 in post monsoon respectively. All the values obtained are

much higher than the limits. High TDS increase density of water, decrease solubility of gases like oxygen and ultimately make the water unsuitable for drinking [18]. High TDS level(>500mg/L) result in excessive scaling in water pipes, water heater, boilers, and household appliances [19].

Hardness: Hardness reflects the composite measure of polyvalent cations whereas calcium and magnesium is the primary constituent of hardness [20]. Public acceptability of the degree of hardness may vary considerably from one community to another. Hardness value above 200mg/L is generally unacceptable. There is no recent reliable data on possible adverse effects associated with hardness 200mg/L may cause scale deposition in distribution system as well as increase soap consumption. Hardness of studied ground water samples varied from 186.5 mg/L at S7 to 718.4 mg/L at S26 in pre-monsoon season,242.9 mg/L at S 21 to 799.9 mg/L in monsoon season and 261.9 mg/L at S 20 to 769.9 mg/L in post-monsoon respectively and most of the values are above the permissible limits of WHO.

Calcium: There is a significant variation in calcium content during the three seasons of investigation in all the sites which varied from 51.0 mg/L at S11 to 96.0 mg/L at S 19 mg/L in Pre-monsoon, 59.0 mg/L at S 21 to 88.0 mg/L at S24 in monsoon season and 51 mg/L at S11 to 80.0 mg/L at 19 in Post monsoon respectively. According to Bureau of Indian Standards [21], standard value for calcium is 75 mg/L and can be relaxed up to 200 mg/L. The higher value of calcium registered during the study period may be due to the influx of industrial waste and sewage to the river water . In estuarine water, the variation of concentration of calcium is quite significant due to land drainage, high rates of biological uptake, and precipitation and dissolution process characteristics of shallow system [22]. More than 50% of present water samples exceed the permissible limits.

Magnesium: As per BIS [21], prescribed standard limit for magnesium is 30-70 mg/L and hence the observed values were beyond the permissible limit. Calcium content of Mudhol taluka ranged from 48.0 mg/L at S13 to 86.o at S 9 in pre-monsoon, 55.0 mg/L at S 21 to 92.0 mg/L at S9 mg/L in monsoon season and 50.0 mg/L at S 17 to 98.0 mg/L at S 5 in post monsoon season respectively. As estuaries receive inputs from multiple sources of organic and inorganic matter such as materials exported from agricultural, urban development through drainage basin in to the river and intrusion of marine water from ocean during high tidal periods which contain multiple

ionic sources such as Ca^{+2}, Mg^{+2}, Cl^- etc may increase the magnesium content in the study sites [23].

Sulphate: The sources of sulphate in underground waters may be rocks, geological formation, and so on. Excess sulphate has a laxative effect, especially in combination with magnesium and/or sodium. Sulphates exist in nearly all natural waters, the concentrations varying according to the nature of the terrain through which they flow. They are often derived from the sulphides of heavy metals (iron, nickel, copper and lead). Iron sulphides are present in sedimentary rocks from which they can be oxidised to sulphate in humid climates; the latter may then leach into watercourses so that ground waters are often excessively high in sulphates[24]. As magnesium and sodium are present in many waters, their combination with sulphate will have an enhanced laxative effect of greater or lesser magnitude depending on concentration. The utility of water for domestic purposes will therefore be severely limited by high sulphate concentrations, hence the limit of 200 mg/dm^3 SO_4^{2-} [24]. The sulphate contents of all the water samples ranged from 140mg/L at S21 to 178mg/L in Pre-monsoon,141mg/L at S49 to 187mg/L at S9 in monsoon season season and 139mg/L to 166mg/L in post-monsoon season respectively. The sulphate contents of all the water samples fall below the MPL (200 mg/dm^3).

Conclusion

In this case study, different physico-chemical parameters were successfully applied and compared with the respective standards to monitor the water quality of Mudhol taluaka of Bagalkot district ,Karnataka India . Water analysis of pH, conductivity, TDS, hardness, calcium, magnesium and sulphate , are the most important parameters represent the pollution. status of the water. The pollutants are due to the release of effluents from several sources into the estuary, which causes significant changes in the quality of water and pose some deleterious effect to the mangrove ecosystem in a long run. The immediate need is to maintain existing sewage treatment plants so that effluent discharge has a minimum of suspended solids. As a result, it is essential that Mudhol taluka environment monitoring is urgently required.

Acknowledgements: Authors are grateful to the UGC New Delhi for providing financial support to carry out this study. We express our deep sense of gratitude to BLDE management Vijayapur, Principal and HOD Chemistry for their help and cooperation. We are grateful to the authorities permitting us to carry out the present study.

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Table.1 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Pre Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.02	2543	1547.1	559.5	70	65	141
2	Sameerwadi public bore well	7.89	2335	1125.2	413.3	60	65	150
3	Belagali public bore well	6.92	2254	1061.0	399.2	55	64	142
4	Mugalkod public tap	7.16	2289	1008.2	372.9	62	65	150
5	Budni PM 1 public bore well	7.21	2312	1002.0	368.2	61	67	156
6	Budni PM 2 public bore well	7.12	2485	1053.0	385.9	60	67	145
7	Nagaral public bore well	7.33	2588	1014.6	389.8	61	65	141
8	Dhavaleshwar public bore well	7.05	2443	1108.2	405.4	63	61	136
9	Sanganatti public bore well	7.55	2537	1408.6	758.3	71	80	164
10	Vajjarmatti public bore well	7.25	2004	869.3	369.2	56	58	141
11	Lokapur public bore well	8.02	1919	638.3	276.5	51	55	148
12	Nandaganv public bore well	7.33	2413	1184.6	437.6	62	60	150
13	Akkimaradi public bore well	7.45	2165	878.8	303.8	52	48	145
14	Sayadapur Public bore well	7.11	2198	965.4	332.6	60	55	143
15	Mugalkod public bore well	7.31	2445	1024.6	423.8	65	69	161
16	Kullalli public tap	7.18	2389	1085.8	399.3	62	54	151
17	Mudhol public bore well budni road	7.33	2025	1007.8	277.8	60	51	144
18	Mudhol public bore well bilagi road	7.22	2115	920.1	362.2	58	52	150
19	Mudhol public bore well near buss stand	7.47	2652	1381.5	769.9	86	70	171
20	Alagundi BK public bore well	6.48	2134	401.9	261.9	58	51	142
21	Malapur public tap	8.02	2174	1009.5	390.5	52	46	140

22	Shirol public Bore well	8.01	2256	1004.5	385.9	57	58	154
23	Shirol public tap water	7.80	2301	1016.4	395.9	52	54	152
24	Konnur public Bore well	7.43	2585	1087.4	418.4	72	69	170
25	Mantur public Bore well	7.59	2557	1006.4	389.4	56	60	141
26	Machaknur public Bore well	7.16	2684	1107.4	413.5	69	70	162
27	Timmapur public Bore well	7.29	2548	1005.3	387.2	66	61	145
28	Jeergal public Bore well	8.04	2454	989.3	385.6	66	61	152
29	Chichakandi public Bore well	7.66	2401	1008.8	375.4	61	52	141
30	Kasabajambagi public Bore well	7.15	2421	987.5	370.5	63	56	150
31	Malali public Bore well	7.75	2568	1105.4	389.7	65	54	153
32	Halagali public Bore well	7.39	2424	1007.3	385.3	60	51	145
33	Kataraki public Bore well	7.14	2489	1022.3	395.5	57	52	145
34	Muddapur public Bore well	7.72	2398	996.4	386.4	61	55	150
35	Bisanal public Bore well	8.02	2454	1007.2	384.7	64	66	161
36	Mahalingapur public Bore well	7.69	2415	1015.5	390.4	70	67	160
37	Madhabanvi public Bore well	7.59	2511	1084.3	416.6	63	62	152
38	Marapur public Bore well	7.82	2465	992.9	381.7	58	62	153
39	Hebbal public Bore well	7.37	2145	901.4	378.4	62	54	145
40	Soraganvi Bore well	7.07	2289	985.9	422.3	68	63	158
41	Alagur public Bore well	8.05	2101	988.5	418.7	60	54	141
42	Chikkalgundi public Bore well	7.77	2135	1037.4	459.7	62	67	161
43	Chikkur public Bore well	7.69	2391	1086.3	416.3	71	73	164
44	Bantanur public Bore well	8.01	2123	903.8	389.6	61	63	165
45	Bannurpublic Bore well	7.72	2566	1104.5	479.2	67	70	167

46	Rugi public Bore well	8.01	2167	1017.5	470.3	70	67	160
47	Jaliber public Bore well	7.78	2685	1102.3	479.5	75	72	161
48	Metagudda public Bore well	7.57	2402	1104.5	423.6	70	65	160
49	Dadanatti public Bore well	7.82	2275	1026.4	403.4	63	60	150
50	Baragi public Bore well	7.77	2362	1109.6	475.5	65	63	156

Table.2 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.44	2968	1897.2	599.6	85	76	168
2	Sameerwadi public bore well	8.01	2755	1478.5	475.2	72	81	169
3	Belagali public bore well	7.52	2665	1309.2	419.6	75	79	169
4	Mugalkod public tap	7.36	2589	1206.6	482.5	79	79	169
5	Budni PM 1 public bore well	7.78	2654	1216.2	618.3	72	78	174
6	Budni PM 2 public bore well	7.61	2765	1332.1	495.2	79	78	171
7	Nagaral public bore well	7.81	2858	1252.3	398.6	79	79	169
8	Dhavaleshwar public bore well	7.46	2745	1208.6	455.9	77	79	156
9	Sanganatti public bore well	7.91	2869	1599.8	798.5	81	92	187
10	Vajjarmatti public bore well	7.71	2226	988.8	408.3	76	77	168
11	Lokapur public bore well	8.20	2229	995.6	420.4	66	65	166
12	Nandaganv public bore well	8.13	2868	1325.4	504.2	76	74	169
13	Akkimaradi public bore well	7.65	2525	1208.5	436.5	66	68	169
14	Sayadapur Public bore well	7.62	2435	1189.6	411.5	69	71	168
15	Mugalkod public bore well	7.62	2798	1318.5	469.5	79	77	177
16	Kullalli public tap	7.61	2745	1215.5	453.4	75	69	166
17	Mudhol public bore well budni road	7.79	2305	1122.5	438.6	66	62	161
18	Mudhol public bore well bilagi road	7.46	2758	1325.6	548.9	82	72	179
19	Mudhol public bore well near buss stand	7.57	2892	1481.7	809.9	89	76	188
20	Alagundi BK public bore well	7.12	2547	1152.6	461.7	69	68	162
21	Malapur public tap	8.02	2454	1118.6	428.9	63	62	168
22	Shirol public Bore well	8.12	2534	1107.8	409.2	68	72	170

23	Shirol public tap water	8.01	2589	11 26.5	417.5	69	71	168
24	Konnur public Bore well	7.72	2945	1408.6	802.6	87	88	184
25	Mantur public Bore well	7.99	2864	1325.3	732.8	70	71	168
26	Machaknur public Bore well	7.42	2894	1309.5	765.8	82	86	175
27	Timmapur public Bore well	7.51	2792	1238.4	705.3	77	79	170
28	Jeergal public Bore well	8.10	2698	1123.5	585.1	70	69	166
29	Chichakandi public Bore well	7.98	2698	1178.7	595.8	73	68	168
30	Kasabajambagi public Bore well	7.52	2723	1318.2	767.2	68	70	170
31	Malali public Bore well	8.31	2888	1472.5	785.9	72	73	172
32	Halagali public Bore well	7.68	2712	1377.5	702.5	68	69	163
33	Kataraki public Bore well	7.45	2898	1478.5	809.6	74	71	168
34	Muddapur public Bore well	8.12	2768	1266.5	715.9	71	70	168
35	Bisanal public Bore well	8.01	2712	1212.3	685.8	69	65	169
36	Mahalingapur public Bore well	7.57	2755	1243.2	695.8	71	75	171
37	Madhabanvi public Bore well	7.89	2889	1153.4	589.7	73	76	172
38	Marapur public Bore well	8.08	2724	1222.6	678.8	69	71	167
39	Hebbal public Bore well	7.77	2415	1185.5	525.6	62	63	168
40	Soraganvi Bore well	7.38	2536	1110.2	495.6	69	73	169
41	Alagur public Bore well	8.15	2401	1125.5	528.7	67	62	159
42	Chikkalgundi public Bore well	7.79	2335	1097.8	469.5	69	68	165
43	Chikkur public Bore well	7.78	2510	1136.7	543.8	73	74	169
44	Bantanur public Bore well	8.13	2340	1098.9	459.8	68	69	164
45	Bannurpublic Bore well	7.85	2661	1254.8	619.8	68	66	168
46	Rugi public Bore well	7.89	2445	1123.9	547.8	73	68	164

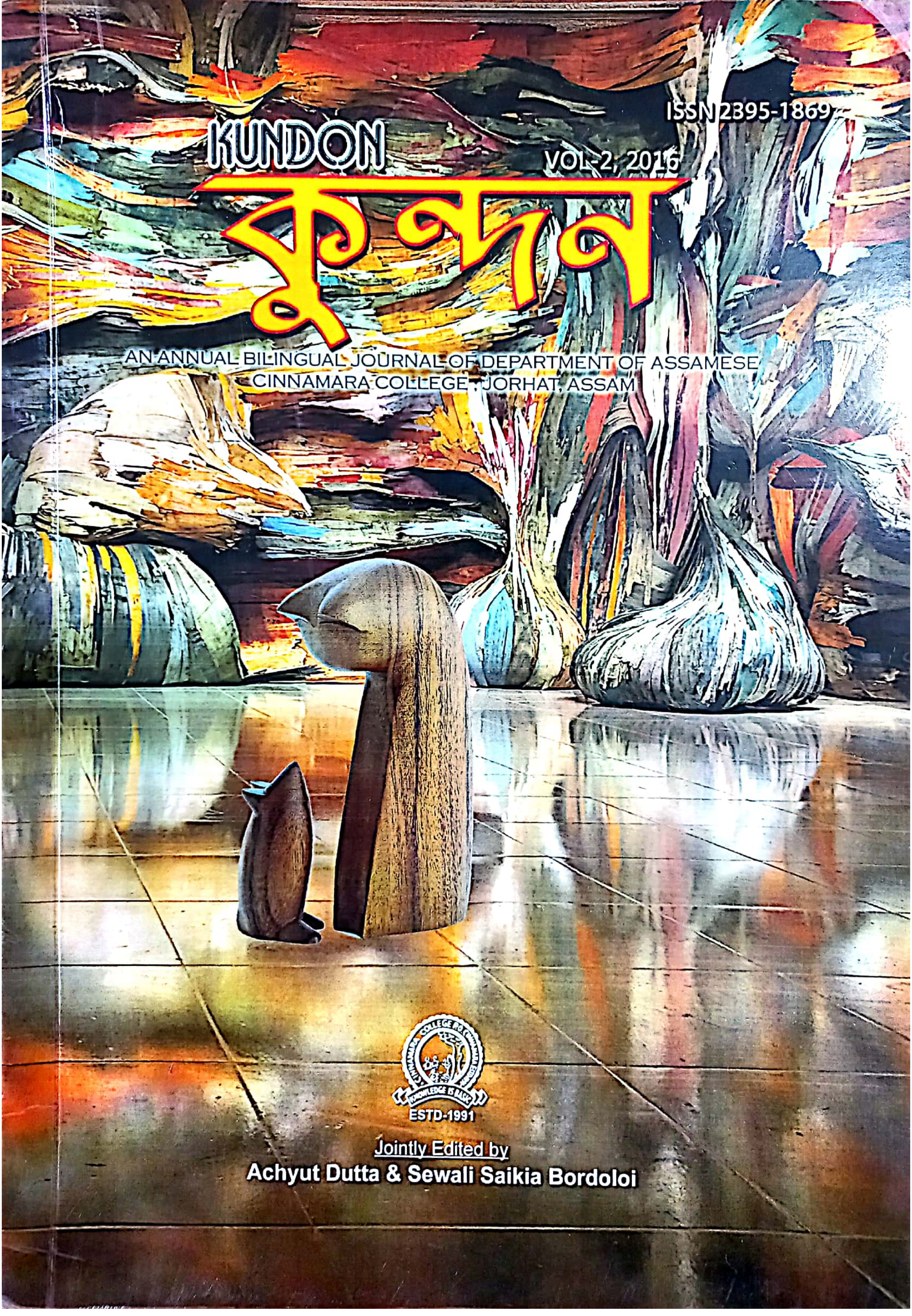
47	Jaliber public Bore well	7.79	2765	1344.8	715.9	71	68	162
48	Metagudda public Bore well	7.79	2512	1228.4	614.7	73	68	160
49	Dadanatti public Bore well	8.11	2414	1120.8	512.5	68	66	161
50	Baragi public Bore well	7.87	2522	1138.8	548.7	69	72	169

Table.3 Physico-Chemical Parameters in the different locations of Mudhol taluka in Bagalkot District.(Post Mansoon)

S No	Area of Samples collected	pH	EC	TDS in ppm	Hardness in ppm	Ca	Mg	SO_4
1	Kesargoppa public bore well	7.12	2814	1797.2	576.8	78	73	166
2	Sameerwadi public bore well	7.41	2587	1289.6	447.1	60	71	153
3	Belagali public bore well	7.11	2489	1145.3	355.4	57	65	156
4	Mugalkod public tap	7.05	2404	1031.4	389.9	67	68	155
5	Budni PM 1 public bore well	7.11	2422	1049.3	565.4	63	98	160
6	Budni PM 2 public bore well	7.05	2581	1191.3	438.6	58	67	156
7	Nagaral public bore well	7.11	2689	1100.6	331.5	60	65	150
8	Dhavaleshwar public bore well	7.12	2509	1103.3	405.5	65	67	140
9	Sanganatti public bore well	7.32	2687	1401.5	706.6	70	78	160
10	Vajjarmatti public bore well	7.15	2009	1145.6	455.6	56	61	142
11	Lokapur public bore well	7.59	2045	938.4	459.8	52	53	141
12	Nandaganv public bore well	7.37	2671	1201.2	535.3	61	64	150
13	Akkimaradi public bore well	7.15	2315	1217.9	556.8	53	56	151
14	Sayadapur Public bore well	7.27	2249	1207.7	550.6	56	57	143
15	Mugalkod public bore well	7.32	2585	1088.4	426.7	68	65	156
16	Kullalli public tap	7.05	2520	1089.9	521.5	62	56	148
17	Mudhol public bore well budni road	7.32	2105	930.6	371.7	54	50	141
18	Mudhol public bore well bilagi road	7.02	2589	1146.8	603.7	70	56	151
19	Mudhol public bore well near buss stand	7.25	2788	1185.9	774.4	80	65	161
20	Alagundi BK public bore well	7.02	2358	1186.4	525.5	56	54	142
21	Malapur public tap	7.34	2287	1021.4	484.3	53	51	150
22	Shirol public Bore well	7.41	2335	1028.2	488.3	56	60	153

23	Shirol public tap water	7.57	2425	1051.8	471.8	54	61	153
24	Konnur public Bore well	7.33	2734	1326.2	673.8	70	72	170
25	Mantur public Bore well	7.55	2689	1035.5	588.5	58	61	145
26	Machaknur public Bore well	7.12	2735	1115.2	606.4	71	72	155
27	Timmapur public Bore well	7.28	2631	1038.8	544.8	65	68	152
28	Jeergal public Bore well	7.51	2504	1047.3	459.3	61	60	152
29	Chichakandi public Bore well	7.58	2507	1107.9	491.2	61	60	145
30	Kasabajambagi public Bore well	7.12	2536	1046.8	422.8	53	60	150
31	Malali public Bore well	8.01	2701	1178.8	548.4	56	60	153
32	Halagali public Bore well	7.26	2514	1083.4	441.8	55	61	152
33	Kataraki public Bore well	7.11	2716	1087.6	662.4	60	62	151
34	Muddapur public Bore well	7.72	2485	1015.3	395.3	59	61	151
35	Bisanal public Bore well	7.67	2511	1025.5	451.7	51	60	155
36	Mahalingapur public Bore well	7.19	2586	1025.3	531.6	62	65	160
37	Madhabanvi public Bore well	7.59	2604	1084.5	579.2	63	67	155
38	Marapur public Bore well	7.72	2510	1013.7	502.4	57	63	153
39	Hebbal public Bore well	7.32	2211	966.9	378.4	56	65	154
40	Soraganvi Bore well	7.10	2374	1022.8	364.2	55	61	151
41	Alagur public Bore well	7.78	2205	1015.8	361.8	54	51	140
42	Chikkalgundi public Bore well	7.55	2184	959.5	345.6	52	60	145
43	Chikkur public Bore well	7.54	2322	1001.8	509.7	60	62	150
44	Bantanur public Bore well	7.72	2175	869.5	311.4	52	53	145
45	Bannurpublic Bore well	7.57	2478	1087.1	468.4	52	54	151
46	Rugi public Bore well	7.61	2279	950.7	375.7	62	54	141

47	Jaliber public Bore well	7.51	2584	1021.7	472.7	68	60	146
48	Metagudda public Bore well	7.47	2304	1021.5	459.8	62	51	140
49	Dadanatti public Bore well	8.01	2292	1066.8	410.4	61	59	139
50	Baragi public Bore well	7.55	2389	1065.9	482.8	68	59	155



ISSN 2395-1869

KUNDON

VOL-2, 2016

কুন্দন

AN ANNUAL BILINGUAL JOURNAL OF DEPARTMENT OF ASSAMESE
CINNAMARA COLLEGE, JORHAT, ASSAM

KNOWLEDGE IS BASIC
ESTD-1991

Jointly Edited by
Achyut Dutta & Sewali Saikia Bordoloi

Vol-2, 2016
ISSN:2395-1869

কুন্দন
KUNDON

An Annual Journal of Department of Assamese, Cinnamara College, Jorhat, Assam

Jointly edited by
Achyut Dutta
Sewali Saikia Bordoloi

Associate Editors
Dr. Bornali Borthakur
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ESTD-1991

Cinnamara College Publication

Reimagining the myths: Analysis of the writings of Contemporary Indian writers

■ Siddheswar Kamati

Introduction:

Indian mythology with its rich line of stories and archetypical characters has been an area of interest among authors across the globe; be it classical authors who write about Indian Gods with their larger than life image or recent attempts by Indian authors to humanize them. The idea of rewriting a God has almost always been accepted by the readers as well as the publishers. The condition however is that the interpretation is not very deviant from the common belief as was the case with Wendy Doniger's "The Hindus-An alternative History" which had to be withdrawn from the market owing to the series of protests against it.

The concept of interpretation in Indian mythology is not entirely new. The two pillars of mythological literature are 'Sruti' and 'Smriti'. Sruti refers to the divine literature which is believed to have had no human intervention in its making . Smriti on the other hand is what is remembered by the sages and put to words, needless to say with their own subjective interpretations . Although Sruti enjoys a greater status than Smriti when it comes to authority, nonetheless, the concept of remembered texts passed on to generation by sages has been there in Indian mythology.

The attempt to retell mythology can have several approaches to it. The televised versions of Ramananad Sagar's Ramayana and Mahabharat portrayed Gods in the similar larger than life image which made them extremely popular with the Indian masses at that time. The thrust in the more recent times, however, has been to respectfully humanize the Gods, thus bringing them closer to people. The same can be seen in Amish Tripathi's Shiva Trilogy.

The trend was started by Ashok Banker through his series of 8 books where he rewrote the story of Ramayana. A more intellectual and insightful edge was added to it by Devdutt Pattanaik who also works as a leadership consultant, whose work focuses on deriving management insights from mythology to reveal a very Indian approach to modern business.

The idea that Amish Tripathi's Immortal of Meluha was rejected 20 times by publishers before indicates that there probably wasn't an established market for that kind of writing. Or possibly there were doubts about the acceptance of text that humanizes Shiva the God's God. But the series turned out to be a great success. So much so that it became the first book series to have music album dedicated to it. This is indicative of a trend where readers are willing to accept and appreciate sensible interpretations.

Background of the Writers:

Devdutt Pattanaik

Devdutt Pattanaik is a famous author and mythologist. Devdutt's parents migrated from Odisha to Mumbai over 50 years ago.

He was born and brought up in Mumbai, and he currently lives in Mumbai. He has two sisters, and two nephews. He was a trained medical practitioner before he left it for writing. The celebrated writer has worked for over 15 years in the healthcare industry, with companies such as Apollo Health Street and Sanofi Aventis, before joining Ernst & Young as Business Advisor.

Devdutt has also worked as leadership consultant, deriving management insights from mythology to reveal a very Indian approach to modern business. He has written over 30 books, with best-sellers like Myth = Mithya, Business Sutra, The Pregnant King, and Jaya: An illustrated retelling of the Mahabharata.

His books have been translated in multiple Indian languages like Hindi, Tamil, Telugu, Gujarati and Marathi. He continues to study and write on mythological stories and symbols, alongside drawing insights about business, leadership, and modern life. He also writes on management and culture regularly in The Economic Times (Corporate Dossier supplement), Mid-Day, Speaking Tree and the DailyO (India Today website).

Devdutt has also worked as the Chief Belief Officer of Future Group and is now a much sought-after public speaker and culture consultant for corporations and business leaders. Additionally, Reliance consults him on matters related to culture and Star TV on various mythological serials.

Amish Tripathi

Amish Tripathi is an IIM (Kolkata)-educated boring banker turned happy author. The success of his first book, The Immortals of Meluha of the Shiva Trilogy, encouraged him to give up a fourteen-year-old career in financial services to focus on writing. He is passionate about history, mythology, philosophy and is an ardent admirer of the Lord Shiva.

Amish has most recently written the Shiva Trilogy which includes The Immortals of Meluha, The Secret of the Nagas & The Oath of the Vayuputras, which has sold over 2 million copies in India since 2010, grossing over Rs 500 million and making the Shiva Trilogy the fastest selling books series in Indian history. The books that he plans to write in the future are also in the areas of mythology & history.

He has over 14 years of experience in the financial services industry. His last job was as National Head – Marketing & Product Management and Member of the Senior Management Committee at IDBI Federal Life Insurance.

The Tribal Warrior versus The Earth's Daughter

The Immortals of Meluha is Amish's first book in the series of Shiva Trilogy and Devdutt's Sita is a version of Ramayan through Sita's eyes. Taking a close look at both the books gives a rich insight into the writing styles of the authors. It also helps in understanding how Amish's writing is different from Devdutt's.

Sita is a version of Ramayan, a retelling, a very small part of the huge texts and interpretations written around the legendary king Ram and his wife, the Queen Sita. Devdutt, right in the prologue of the book states this fact. The author makes no assertions as to being able to cover all that is said and known about the Goddess in the book, but humbly states the story as he could gather from the various interpretations that he has read. "Within all these stories is the truth. Who knows it all? Varuna has but a thousand eyes; Indra, a hundred; You and I only two." (Pattanaik 2013).

The high note of the book Sita is that it has information tables across all chapters. These tables enlist views that are known and written about the various characters and incidents of Ramayan across India and beyond. For instance, the name of Sita's mother is different across different interpretation of Ramayan (Pattanaik 2013). Although the author chooses to take up one name, and consequently one version of it, he mentions the rest in the information tables duly. This reflects on the authors understanding of Smriti which forms the pillar of Hindu mythology and literary texts. It also shows the author's reluctance to project a personal favorite version among the options available. The treatment of the protagonist Sita is very objectively done by the author.

On the other hand, Amish's Immortals of Meluha reflects the author's personal admiration for the Lord by the way he characterizes Shiva, the tribal warrior. The story entails how a human of flesh and blood becomes Godlike through his deeds. Despite of the author's personal sentiments, he tries to keep the protagonist as human as possible to the point where Shiva introspects about the mistakes that he made in his past life and his total reluctance to be called the chosen Neelkanth, the Destroyer of Evil. "I don't deserve any destiny. If these people knew of my guilt, they would stop this bullshit instantly", thought Shiva. (Tripathi 2010)

Interestingly, Amish chose to have his own explanations for the various incidents known about the Lord Shiva. The Neelkanth or the blue neck of Shiva has been explained as the consequence of drinking poison by the Lord as quoted by Dr. K K Aggarwal. The book however calls it the consequence of drinking a life giving potion called Somras which eventually turns out to be the evil that the protagonist would fight against. There isn't a major diversion in what is already known commonly, but Amish has attempted to add his own subjective interpretations to it making the book all the more interesting.

Sita and The immortals of Meluha agreeably fall under the genre of mythology, but the treatment is pretty different. The former is only one character's account of the story, while the latter is more than just mythology. It is fantasy, somehow touching the genre of books written by Paulo Coelho and Dan Brown. As such, an objective comparison between the protagonists of both the plots that is Sita and Shiva would not be possible. However there still are similarities, the most important one being their characterization as a human and not a larger than life God or Goddess. There are no magic spells, curses, boons or any other such mystic qualities about the characters that would make them any less human than Dan Brown's Robert Langdon (protagonist of the fictions Angels and Demons, DaVinci Code and Inferno).

The belief officer and the literary popstar:

Pattanaik is an intellectual, peer acclaimed author whose writing is simple yet insightful. His writing is mostly focused on bringing mythology into lifestyles as far as practical. What is unique about his way of writing is that he chose to retell a story through major characters of mythological texts. His Ramayan is Sita's Ramayan & Hanuman's Ramayan, his Mahabharat is through Jaya's tale of the war (Draupadi's other name). The stories, however, remain more or less the same. Ramayan is still the story of the legendary hero Ram, there are no antagonistic thoughts in Sita's mind against her husband who disowned her because of a petty washer man. There isn't much of fictitious layering in the story which differentiates it from Amish's Shiva Trilogy.

As opposed to the former, Amish has absolutely romanticized Shiva. In the Immortals of Meluha, Shiva is a brave tribal warrior who has no clue about his role as the 'Destroyer of the evil', who falls in love with a woman like any other man and tries to woo her. He becomes the hero that people worship, isn't born with enlightenment. Amish carefully made additions to the already known fact about various Gods for example why Ganesha has an elephant head. There are folklores that say different stories about it but Amish chose his own way of explaining it which makes him stand out.

' Devdutt is a simple story teller who will keep readers turning the pages. He restricts himself to the plot without experimenting much with the characters. His niche is his sheer understanding of the concept which reflects in his writing style which has depth and clarity of thought. Amish on the other hand has a flamboyant flair for writing. His writing has a modulation of high and low notes. No wonder the Oath of the Vayuputra was pre-ordered by readers out of anticipation. Although it wasn't as big a success as the previous two books of the trilogy, nonetheless it was widely accepted and appreciated.

According to the Business World, Amish is on his way to becoming the Paulo Coelho of the east. The Hindustan Times already called his Trilogy as India's Lord of the Rings. Additionally, adding much pomp to the fanfare that Amish enjoys, the publication house Westland offered him a sum of 5 crore Indian Rupees for his next book series.

Another point to consider here is that Devdutt wrote over 30 books and is a regular columnist in leading newspapers while Amish's shot to fame is his Shiva Trilogy which made him a literary pop star already. The trilogy has a music album dedicated to it and big film makers are planning to adapt the story to take it on to the silver screen. It will not be wrong to say that while the former is the conscience keeper, the latter is the populist leader. The paths chosen by them are different yet leading to the same destination.

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Journal of Agriculture and Ecology Research International
6(1): 1-8, 2016; Article no.JAERI.21770
ISSN: 2394-1073

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www.sciencedomain.org

Bioindicators: Study on Uptake and Accumulation of Heavy Metals in Plant Leaves of State Highway Road, Bagalkot, India

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Authors' contributions

This work was carried out in collaboration between all authors. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/JAERI/2016/21770
Editor(s):
(1) Alejandro E. Ferrari, Department of Science and Technology, UNQ, Universidad Nacional de Quilmes, Argentina.
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Complete Peer review History: http://sciencedomain.org/review-history/12858

Original Research Article

Received 2nd September 2015
Accepted 10th December 2015
Published 31st December 2015

ABSTRACT

In this study, Caesalpinia (*Caesalpinia pulcherrima*) and grass (*Cyndon dactylon*) was evaluated as the bioindicators of heavy metals such as the Lead (Pb), Copper (Cu), Cadmium (Cd), Manganese (Mn), Zinc (Zn), Chromium (Cr) and Nickel (Ni) contaminated in Bagalkot and along the state high way upto Mudhol. The soil samples at depth (0-20 cm) and caesalpinia and grass leaves were taken from different sampling stations namely Navnagar bypass road (S_1), Gaddanakeri cross (S_2), Tulasigeri (S_3), Kaladagi (S_4), Lokapur (S_5), Chichakhandi (S_6) and Mudhol (S_7). The concentrations of Pb, Cu, Cd, Mn, Zn, Cr and Ni were measured using GBC- 932 plus Atomic Absorption Spectrophotometer (Austrelia). The results of the study shows that the concentrations of heavy metals in caesalpinia ranged from Pb 20.36 to 29.39 µg/gmm, Cu 3.92 – 5.94 µg/gm, Zn 24.40 to 35.7 µg/gm, Cd 1.01 to 1.78 µg/gm, Mn 27.01 to 69.10 µg/gm, Cr 1.20 to 7.8 µg/gm and Ni 7.9 to 13.1 µg/gm. In grass heavy metal ranges between for Pb 20.16 to 28.01, Cu 3.95 to 5.76

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µg/gm, Zn 24.50 to 35.8 µg/gm, Cd 1.15 to 1.52 µg/gm, Mn 28.91 to 72.51 µg/gm, Cr 1.28 to 8.0 µg/gm, Ni 8.1 to 15.1 µg/gm. Similarly in roadside soil heavy metal ranges between Pb 81.91 to 139.8 µg/gm, Cu 39.54 to 58.58 µg/gm, Zn 32.29 to 381.54 µg/gm, Cd 1.51 to 2.08 µg/gm, Mn 1257.9 to 2051 µg/gm, Cr 131.9 to 951.2 µg/gm and Ni 69.53 to 108.6 µg/gm. According to these results the concentration of heavy metals in grass was found high as compared to caesalpinia. Thus, compared to the metal accumulation potential grass is said to be heavy metal accumulator. The variation in heavy metal concentrations is due to changes in traffic density and anthropogenic activities. Thus, generally it is considered that grass and caesalpinia are good bioindicators and can be used in air pollution monitoring studies.

Keywords: Heavy metals; bioindicators; accumulation; anthropogenic activities.

1. INTRODUCTION

Environment pollution with toxic metals has increased since increasing industrialization and human activities [1]. Emissions of various pollutants into the atmosphere have a lot of harmful effects on plants growth [2]. Rapid urbanization, unregulated industrialization growing transport intensity and agricultural practices have created heavy metals concentrations in serious stage [3]. Plants have a major contributions in purifying land water and environmental air. Entrance of heavy metals may occur in human and animal food chain as a result of their uptake by edible plant grown in contaminated soil [4]. The toxic and hazardous effects of some heavy metals on human health are very significant and may cause many fatal diseases.

Lead (Pb) is one of the heavy metal that is responsible for anemia, neurological disorder, hyperactivity and changes in blood enzymes in human body [5]. Cadmium (Cd) and Zn are important toxic metals and longtime exposure of which may cause renal, pulmonary, hepatic, skeletal, reproductive and many other carcinogenic effects [6,7]. It is widely recognized that the principal reasons of heavy metals (Pb, Cu and Cd) derived from traffic congestion, long-range transport and household heating [8]. The spreading of contaminants is influenced by meteorological parameters such as rainfall, wind and traffic intensity [4]. The same meteorological conditions affect the concentration of same contaminants in the roadside soil [8]. The traffic density determines the lead level in soil and vegetation [9-11].

Soil samples and vegetation are the most economic and reasonable ways for assessing heavy metal status in the atmosphere [12]. Acacia [13], grass [14], plants [15], and other organisms such as fish [16] have also have been used for monitoring. In order to assess contamination by metals in the vicinity of a highway, several studies have been carried out with the different compartments: Study of global deposits, roadside soil and vegetation [8]. Information on accumulation of heavy metal on roadside soil of this city due to highway traffic and vehicles is very limited [17], but this could be the new threat for agriculture. Determination of heavy metal accumulation in roadside soil may be an index of the environmental pollution of Bagalkot city. Keeping this view in mind, the research was conducted to know the heavy metal accumulation of roadside soil, grass and caesalpinia of Bagalkot city and along the state highway from Bagalkot to Mudhol.

2. MATERIALS AND METHODS

Bagalkot is the city of Northern region of Karnataka at latitude 16° 04^{1} N to 16° 21^{1} North and longitude 75° 26^{1} E to 76° 02^{1} Eastern. The city is suffered from high traffic density caused by vehicles. Grass, caesalpinia and soil were collected during 2013, which were three meters away from the State High way (Fig. 1 and Table 1) passing through Navanagar. Grass and caesalpinia samples were collected from each site at three random spots those were spaced approximately at one meter interval. The leaves were clipped with stainless steel scissors. All the samples of each site were combined to give composite samples of about 300 to 500 gm. The leaves of Grass (*Cyndon dactylon*) and Caesalpinia *(Caesalpinia pulcherrima*) samples were dried at 80℃ for 48 hrs fine by powdered and sieved through 0.2 mm sieve. One gram sample was digested using Gerhardt digestion unit using mixed acid digestion method [18]. The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made upto 100 ml.

Table 1. Sampling stations

Station no.	Sampling station	Nature of stations
Control	**Navanagar (Bagalkot)**	**Unpolluted urban area- vehicular movement is negligible, unpolluted area with less disturbance**
1	Navanagar Bypass road	Vehicular movement is high
2	Gaddankeri cross	Vehicular movement is high. Agricultural fields on either side of the road
3	Tulasigeri	Bricks factories around the Gaddankeri cross, vehicular traffic is high
4	Kaladagi	Vehicular movement is high. Agricultural fields on either side of the road
5	Lokapur	Vehicular movement is high. Agricultural fields on either side of the road
6	Chichakhandi	Vehicular movement is high. Agricultural fields on either side of the road
7	Mudhol	Vehicular movement is high. Agricultural fields on either side of the road

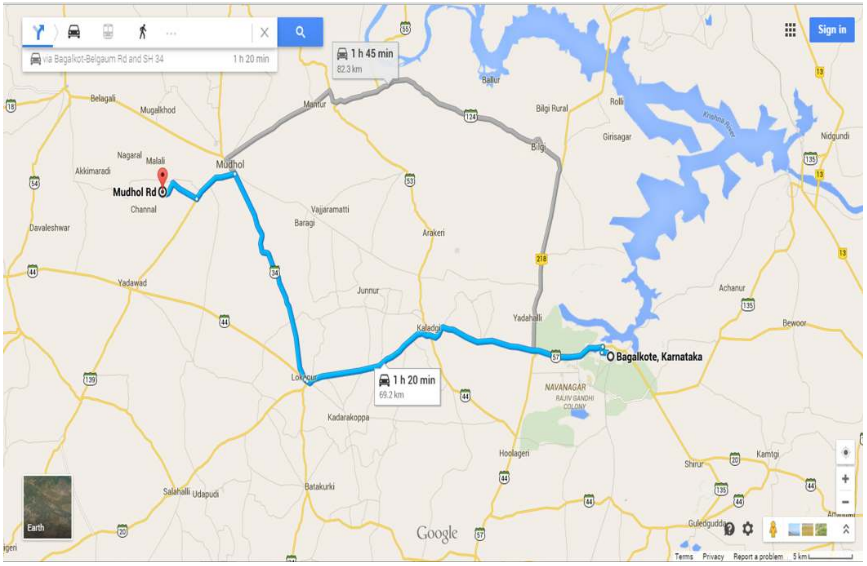

Fig. 1. Map showing the state highway of Bagalkot

Similarly, soil samples were dried, powdered and sieved through 0.2 mm sieve. One gram of sample was digested Gerhardt digestion unit according to Allen et al. [18] method (mixed acid digestion method. The results were in triplicates. The resulting extracts were diluted and filtered through Whattman No 41 paper and made upto 100 ml using double distilled water and analyzed for heavy metals viz Pb (Lead), Cd (Cadmium), Cu (Copper), Zn (Zinc), Mn (Manganese), Ni (Nickel) and Cr (Chromium) with GBC-932 plus Atomic Absorption Spectrophotometer (AAS) (Austrelia)with an air / acetylene flame and metal hollow cathode lamps. Respective wavelengths were used for the estimation of solutions for heavy metals were purchased from Siscochemical Laboratory Bombay (1000 mg/l). For Cd 228.8 nm, Pb 217.0 nm, Ni 232.0 nm, Cu 324.7 nm, Zn 213.9 nm, Mn 279.5 nm and Cr 221.8 nm filters have been used for the estimation using AAS. The working standards were prepared by serial dilution of standard stock solutions and were used for the calibration of the instrument [18].

3. RESULTS AND DISCUSSION

Environmental pollution with toxic metals has increased dramatically since the increasing of vehicular exhausts [19]. The pollution by heavy metals such as Lead, Cadmium, Nickel, Chromium etc is a problem of concern [20]. So it is now necessary to conduct this study and to determine the kinds of environmental pollution and how for these exhibit and act as an efficient bioindicator in reducing the degree of pollution in the environment. The samples were collected along the state highway between Bagalkot to Mudhol for the estimation of heavy metals (Fig. 1). Correlation coefficient of heavy metals in roadside soil, grass and caesalpinia plant samples are given in the Tables 3 and 4. The analysis showed high levels of heavy metals in the leaves of caesalpinia and grass collected from the polluted as compared to less polluted sites of the city (Control).

The ranges and arithmetic mean of heavy metal concentration of soil, grass and caesalpinia samples of state high-way and control sites are presented in the Table 2.

Lead is one of the major heavy metal and is considered as an environmental toxic pollutant [21]. Lead is considered as more toxic pollutant which brings about many physiological disorders. The main sources of lead are exhaust fumes of automobiles, chimneys of factory, roadside vehicles pollution [22]. The results shows that soils tend to accumulate more Pb then grass and caesalpinia leaves. The highest Pb level found in the soil (roadside) was 139.8 µg/gm, in grass it was 28.01 µg/gm, similarly in caesalpinia leaves it was found that 29.39 µg/gm. The mean soil Pb level was 95.71 µg/gm indicated considerable contamination of metal in the roadside environment; however, the control soil has a baseline level of 70.50 µg/gm. The results of our analysis represents, there should be significant differences for lead between sampling sites in control and polluted areas. The lead is rapidly washed onto the soil by rain water from the surface also by the death and decomposition of the plant [23,24]. Many literatures have notified the contents of heavy metals were higher in plant samples collected along the roadside of highways [8].

Copper is also one of the major heavy metal considered as an environmental pollutant. Copper is a micronutrient but toxic when it is in excess concentration. The source of copper being due to corrosion of metallic parts of cars derived from engine wear, brushing and bearing metals [25]. The mean Cu level in roadside soil (49.71 µg/gm) found to be much higher than the grass (4.87 µg/gm) and caesalpinia (4.70 µg/gm).

The main source of Zn on the roadside is because of automobile traffic i.e break lining looses of oil and cooling liquid [26]. Arithmetic mean of Zn of the roadside soil from Bagalkot to Mudhol state highway owes relatively high level of 188.31 µg/gm with a range of 32.29 – 381.54 µg/gm. the range of Zn 24.40 – 35.70 µg/gm in caesalpinia and grass 24.50 – 35.8 µg/gm. however, the Zn content in the test plant samples of polluted area are below the allowed limit (15 – 100 µg/gm) [18].

The main sources of environmental cadmium pollution are vehicle wheels, mineral oils increases Cd levels of environment and plants [27]. Cd dispersed in the natural environment through anthropogenic activities as well as natural rock mineralization process and thus, plants can easily absorbs Cd from the soil and also transport to the shoot levels. Cadmium induces complex changes in plants genetical, physiological and biochemical levels. The values were found little higher than allowed limit (1 µg/gm) in plants, i.e the Cd level in roadside soil averaged about 2.0 µg/gm and was observed that Cd was the lowest among the seven metals tested. The mean Cd in caesalpinia was 1.41 µg/gm and in grass, it is found to be 1.57 µg/gm. These findings were in confirmation with Shafia et al. [28].

From the results it was found that the soil, grass and caesalpinia contained high level of Manganese than other limits. Roadside soil, grass and caesalpinia had average 1528.34 µg/gm, 56.606 µg/gm and 56.10 µg/gm respectively. The attribution of Mn content is the lithogenic factor apart from vehicular pollution [29].

Chromium is considered as a serious concern with respect to health of biotics particularly in detrimental to plant growth and development. Cement, limestone industries are the major causes for the high influx of chromium into the atmosphere [29]. Significant differences in our analysis for chromium in soil and in plant samples are found. Chromium level was too high in roadside soil (315.54 µg/gm against control 110.41 µg/gm. In caesalpinia it was found to be 4.61 µg/gm, in grass it is found that 4.90 µg/gm against control (zero). Thus, the Cr content in soil and test plant samples of polluted area are above the maximum allowed limit (soil- 10-200 µg/gm, plant- 0.05-0.5 µg/gm).

Table 2. Metal accumulation profile in caesalpinia, grass and soil

S. no	Heavy metals	Control (µg g-1 dry wt.)	Roadside Caesalpinia (µg g-1 dry wt.)		Roadside grass (µg g-1 dry wt.)		Control (µg g-1 dry wt.)	Roadside soil (µg g-1 dry wt.)	
			Range	**Mean ± SE**	**Range**	**Mean±SE**		**Range**	**Mean± SE**
1	Lead	18.46	20.36-29.39	23.73±1.84	20.16-28.01	23.736±1.84	70.50	81.91-139.8	95.71±8.71
2	Copper	2.15	3.92-5.94	4.70±0.35	3.95-5.76	4.87±0.35	34.91	39.54-58.58	49.71±3.51
3	Zinc	16.19	24.40-35.7	32.84±3.10	24.50-35.8	32.87±3.11	29.84	32.29-381.54	188.3±54.28
4	Cadmium	0.82	1.01-1.78	1.41±0.08	1.15-1.52	1.571±0.082	2.16	1.51-2.08	2.0±0.19
5	Manganese	15.72	27.01-69.10	56.10±7.30	28.91-72.51	56.606±7.36	1254.1	1257.9-2051.5	1528.3±26.5
6	Chromium	N.D	1.20-7.8	4.61±2.20	1.28-8.00	4.90±2.23	110.41	131.9-951.2	315.54±2.46
7	Nickel	6.70	7.9-13.1	9.10±1.40	8.1-15.1	10.51±1.411	69.38	69.53-108.6	85.91±5.91

ND- Not detectable; Mean values ± standard error

Table 3. Correlation coefficient of heavy metals in roadside soil and grass

S. no.	Metal	r. value
1	Lead	0.628*
2	Copper	0.481*
3	Zinc	0.829*
4	Cadmium	0.748*
5	Manganese	0.529*
6	Nickel	0.331*
7	Chromium	0.215*

r= 0.60 and above have significant correlation

Table 4. Correlation coefficient of heavy metals in roadside soil and caesalpinia

S. no.	Metal	r. value
1	Lead	0.627*
2	Copper	0.480*
3	Zinc	0.824*
4	Cadmium	0.740*
5	Manganese	0.520*
6	Nickel	0.321*
7	Chromium	0.210*

r= 0.60 and above have significant correlation

Nickel is a micronutrient required at very low concentration by the plants normally in Ni^{+2} state, at high concentration Ni inhibits plant growth. The maximum Ni content was found 10.5 µg/gm in grass than caesalpinia with 9.10 µg/gm. Generally it is concluded that Ni content in test plant samples of polluted area are higher than the normal values (0.1 – 5.0 µg/gm) in plants [18].

Simple correlations ($r > 0.60$) between the metal Pb, Cu, Ni, Mn, Fe, Zn and Cd were calculated and are given in the Tables 3 and 4. Significant correlations between the metal levels in roadside soil, caesalpinia and grass were found in Zn, Cd and Ni ($r > 0.06$). It may be indicating the bioconcentration of these metals in soil, grass and caesalpinia, in addition to aerial deposition. This may attributed to the favorable root environment [30] i.e soil conditions might have favored their absorption. Correlations in case of chromium, nickel, manganese and copper contents between soil, grass and caesalpinia were low due to low bioavailability of these metals owing to unfavorable root environment. Whatever excess content of these metals found in grass and caesalpinia was presumed to be due to the aerial decomposition contributed by motor vehicles.

Thus, the order of increment of heavy metals in roadside soil is as follows: Mn > Cr > Zn > Pb > Ni > Cu > Cd, whereas in grass: Mn> Zn> Pb> Ni> Cr> Cu> Cd and in caesalpinia: Mn>Zn > Pb> Ni> Cu> Cr > Cd. The elevated levels of heavy metals in the roadside soil, grass and caesalpinia is an evidence of airborne pollutants of roadside environment along the state high way of Bagalkot to Mudhol. Soils due to their cation exchange capacity (CEC), complexing organic substances, oxides and carbonates, have high retention capacity for the heavy metals [31]. Thus, contamination levels increase continuously as long as the nearby sources remain active. During the last decade, the Bagalakot to Mudhol state high way has witnessed sharp increase in vehicle number due to urbanization. Similar observation in Caesalpinia in Madhurai city of southern region of Tamil Nadu [32].

In soil, the lesser mobility of metals and its accumulation on a long-term basis, leads to overall higher contamination level of metals; whereas, in roadside grass, caesalpinia it represents more accumulation due to turnover of plant materials (like new growths, the senescence followed by abscission of old parts) and meteorological influences [33]. Thus, the study of metal concentration of both roadside soil, grass and caesalpinia reflects the extent of aerial contamination of the roadside environment. The penetration of heavy metals into the food chains due to vehicular emissions may cause a long- range ecological and health hazard.

The results of our study indicate that the concentration of heavy metals such as Pb, Cd, Mn, Ni, Cu and Cr from the traffic area is an indicative of anthropogenic pollution.

4. CONCLUSION

It was concluded that with an increase in the amount of heavy metals in soil and their uptake by plants also increase. The mobility of heavy metals are highly translocated from soil to plant leaves in all the sampling sites. According to our study grass shows slight greater accumulation potentiality than caesalpinia. High metal concentrations in plants are contained in urban and highway roadsides due to the anthropogenic activities in addition to the traffic density. The heavy metal concentration was maximum in the study area along the roadside of Bagalkot to Mudhol. Caesalpinia is widely distributed at Bagalkot (Navanagar) is used as roadside ornamental plant and the grass is the good food for grazing animals. In accordance with the data presented here grass and caesalpinia possess all characteristics and are selected as bioindicators.

There is also a need for enforcement of regulations to control environmental pollution. Public participation, non-governmental organization and civic agencies of the government required collective approach towards the solution. Continuous air monitoring for one or more pollutants is an absolute necessity for completing a diagnosis of pollutant level in the air, water and soil environment. Most importantly, a network of monitoring stations throughout the country would be helpful to measure the current pollutant level. Accumulation of air monitoring data will provide the criteria needed for establishing air quality standards.

ACKNOWLEDGEMENT S

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi (Karnataka), Principal, JSS College Dharwad and to the Chairman, PG Department Botany, Karnatak University, Dharwad (Karnataka) for providing necessary facilities to carry out research work.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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Peer-review history:
The peer review history for this paper can be accessed here:
http://sciencedomain.org/review-history/12858

Journal of Agriculture and Ecology Research International
6(1): 1-8, 2016; Article no.JAERI.21770
ISSN: 2394-1073

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Bioindicators: Study on Uptake and Accumulation of Heavy Metals in Plant Leaves of State Highway Road, Bagalkot, India

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Authors' contributions

This work was carried out in collaboration between all authors. All authors read and approved the final manuscript.

Article Information

DOI: 10.9734/JAERI/2016/21770
Editor(s):
(1) Alejandro E. Ferrari, Department of Science and Technology, UNQ, Universidad Nacional de Quilmes, Argentina.
(2) Krzysztof Skowron, Department of Microbiology, Nicolaus Copernicus University in Toruń, Collegium Medicum of L. Rydygier in Bydgoszcz, Poland.
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(3) Rajaram Pandurang Dhok, Savitribai Phule Pune University, Pune, India.
Complete Peer review History: http://sciencedomain.org/review-history/12858

Original Research Article

Received 2nd September 2015
Accepted 10th December 2015
Published 31st December 2015

ABSTRACT

In this study, Caesalpinia (*Caesalpinia pulcherrima*) and grass (*Cyndon dactylon*) was evaluated as the bioindicators of heavy metals such as the Lead (Pb), Copper (Cu), Cadmium (Cd), Manganese (Mn), Zinc (Zn), Chromium (Cr) and Nickel (Ni) contaminated in Bagalkot and along the state high way upto Mudhol. The soil samples at depth (0-20 cm) and caesalpinia and grass leaves were taken from different sampling stations namely Navnagar bypass road (S_1), Gaddanakeri cross (S_2), Tulasigeri (S_3), Kaladagi (S_4), Lokapur (S_5), Chichakhandi (S_6) and Mudhol (S_7). The concentrations of Pb, Cu, Cd, Mn, Zn, Cr and Ni were measured using GBC- 932 plus Atomic Absorption Spectrophotometer (Austrelia). The results of the study shows that the concentrations of heavy metals in caesalpinia ranged from Pb 20.36 to 29.39 µg/gmm, Cu 3.92 – 5.94 µg/gm, Zn 24.40 to 35.7 µg/gm, Cd 1.01 to 1.78 µg/gm, Mn 27.01 to 69.10 µg/gm, Cr 1.20 to 7.8 µg/gm and Ni 7.9 to 13.1 µg/gm. In grass heavy metal ranges between for Pb 20.16 to 28.01, Cu 3.95 to 5.76

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µg/gm, Zn 24.50 to 35.8 µg/gm, Cd 1.15 to 1.52 µg/gm, Mn 28.91 to 72.51 µg/gm, Cr 1.28 to 8.0 µg/gm, Ni 8.1 to 15.1 µg/gm. Similarly in roadside soil heavy metal ranges between Pb 81.91 to 139.8 µg/gm, Cu 39.54 to 58.58 µg/gm, Zn 32.29 to 381.54 µg/gm, Cd 1.51 to 2.08 µg/gm, Mn 1257.9 to 2051 µg/gm, Cr 131.9 to 951.2 µg/gm and Ni 69.53 to 108.6 µg/gm. According to these results the concentration of heavy metals in grass was found high as compared to caesalpinia. Thus, compared to the metal accumulation potential grass is said to be heavy metal accumulator. The variation in heavy metal concentrations is due to changes in traffic density and anthropogenic activities. Thus, generally it is considered that grass and caesalpinia are good bioindicators and can be used in air pollution monitoring studies.

Keywords: Heavy metals; bioindicators; accumulation; anthropogenic activities.

1. INTRODUCTION

Environment pollution with toxic metals has increased since increasing industrialization and human activities [1]. Emissions of various pollutants into the atmosphere have a lot of harmful effects on plants growth [2]. Rapid urbanization, unregulated industrialization growing transport intensity and agricultural practices have created heavy metals concentrations in serious stage [3]. Plants have a major contributions in purifying land water and environmental air. Entrance of heavy metals may occur in human and animal food chain as a result of their uptake by edible plant grown in contaminated soil [4]. The toxic and hazardous effects of some heavy metals on human health are very significant and may cause many fatal diseases.

Lead (Pb) is one of the heavy metal that is responsible for anemia, neurological disorder, hyperactivity and changes in blood enzymes in human body [5]. Cadmium (Cd) and Zn are important toxic metals and longtime exposure of which may cause renal, pulmonary, hepatic, skeletal, reproductive and many other carcinogenic effects [6,7]. It is widely recognized that the principal reasons of heavy metals (Pb, Cu and Cd) derived from traffic congestion, long-range transport and household heating [8]. The spreading of contaminants is influenced by meteorological parameters such as rainfall, wind and traffic intensity [4]. The same meteorological conditions affect the concentration of same contaminants in the roadside soil [8]. The traffic density determines the lead level in soil and vegetation [9-11].

Soil samples and vegetation are the most economic and reasonable ways for assessing heavy metal status in the atmosphere [12]. Acacia [13], grass [14], plants [15], and other organisms such as fish [16] have also have been used for monitoring. In order to assess contamination by metals in the vicinity of a highway, several studies have been carried out with the different compartments: Study of global deposits, roadside soil and vegetation [8]. Information on accumulation of heavy metal on roadside soil of this city due to highway traffic and vehicles is very limited [17], but this could be the new threat for agriculture. Determination of heavy metal accumulation in roadside soil may be an index of the environmental pollution of Bagalkot city. Keeping this view in mind, the research was conducted to know the heavy metal accumulation of roadside soil, grass and caesalpinia of Bagalkot city and along the state highway from Bagalkot to Mudhol.

2. MATERIALS AND METHODS

Bagalkot is the city of Northern region of Karnataka at latitude $16^\circ 04^1$ N to $16^\circ 21^1$ North and longitude $75^\circ 26^1$ E to $76^\circ 02^1$ Eastern. The city is suffered from high traffic density caused by vehicles. Grass, caesalpinia and soil were collected during 2013, which were three meters away from the State High way (Fig. 1 and Table 1) passing through Navanagar. Grass and caesalpinia samples were collected from each site at three random spots those were spaced approximately at one meter interval. The leaves were clipped with stainless steel scissors. All the samples of each site were combined to give composite samples of about 300 to 500 gm. The leaves of Grass (*Cyndon dactylon*) and Caesalpinia *(Caesalpinia pulcherrima*) samples were dried at 80℃ for 48 hrs fine by powdered and sieved through 0.2 mm sieve. One gram sample was digested using Gerhardt digestion unit using mixed acid digestion method [18]. The digested material was diluted with double distilled water and filtered through Whattman paper 41 and made upto 100 ml.

Table 1. Sampling stations

Station no.	Sampling station	Nature of stations
Control	**Navanagar (Bagalkot)**	**Unpolluted urban area- vehicular movement is negligible, unpolluted area with less disturbance**
1	Navanagar Bypass road	Vehicular movement is high
2	Gaddankeri cross	Vehicular movement is high. Agricultural fields on either side of the road
3	Tulasigeri	Bricks factories around the Gaddankeri cross, vehicular traffic is high
4	Kaladagi	Vehicular movement is high. Agricultural fields on either side of the road
5	Lokapur	Vehicular movement is high. Agricultural fields on either side of the road
6	Chichakhandi	Vehicular movement is high. Agricultural fields on either side of the road
7	Mudhol	Vehicular movement is high. Agricultural fields on either side of the road

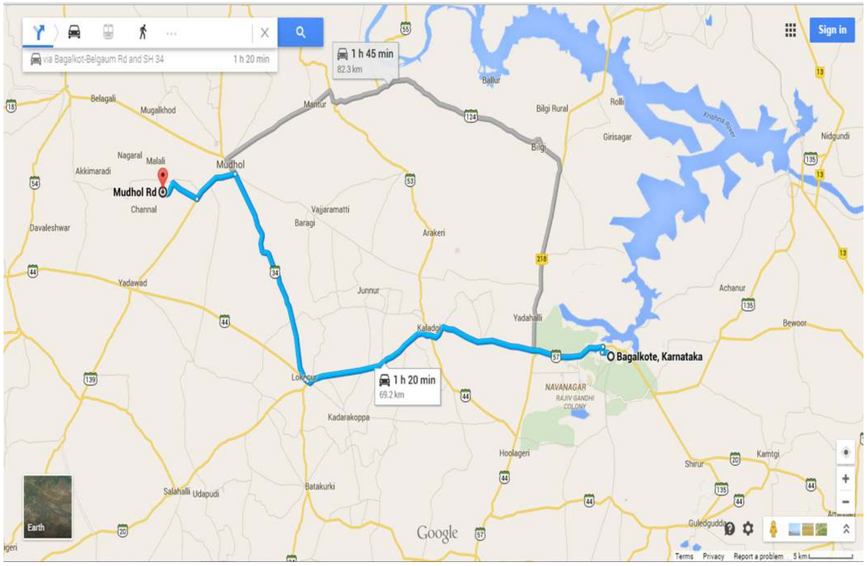

Fig. 1. Map showing the state highway of Bagalkot

Similarly, soil samples were dried, powdered and sieved through 0.2 mm sieve. One gram of sample was digested Gerhardt digestion unit according to Allen et al. [18] method (mixed acid digestion method. The results were in triplicates. The resulting extracts were diluted and filtered through Whattman No 41 paper and made upto 100 ml using double distilled water and analyzed for heavy metals viz Pb (Lead), Cd (Cadmium), Cu (Copper), Zn (Zinc), Mn (Manganese), Ni (Nickel) and Cr (Chromium) with GBC-932 plus Atomic Absorption Spectrophotometer (AAS) (Austrelia)with an air / acetylene flame and metal hollow cathode lamps. Respective wavelengths were used for the estimation of solutions for heavy metals were purchased from Siscochemical Laboratory Bombay (1000 mg/l). For Cd 228.8 nm, Pb 217.0 nm, Ni 232.0 nm, Cu 324.7 nm, Zn 213.9 nm, Mn 279.5 nm and Cr 221.8 nm filters have been used for the estimation using AAS. The working standards were prepared by serial dilution of standard stock solutions and were used for the calibration of the instrument [18].

3. RESULTS AND DISCUSSION

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The ranges and arithmetic mean of heavy metal concentration of soil, grass and caesalpinia samples of state high-way and control sites are presented in the Table 2.

Lead is one of the major heavy metal and is considered as an environmental toxic pollutant [21]. Lead is considered as more toxic pollutant which brings about many physiological disorders. The main sources of lead are exhaust fumes of automobiles, chimneys of factory, roadside vehicles pollution [22]. The results shows that soils tend to accumulate more Pb then grass and caesalpinia leaves. The highest Pb level found in the soil (roadside) was 139.8 µg/gm, in grass it was 28.01 µg/gm, similarly in caesalpinia leaves it was found that 29.39 µg/gm. The mean soil Pb level was 95.71 µg/gm indicated considerable contamination of metal in the roadside environment; however, the control soil has a baseline level of 70.50 µg/gm. The results of our analysis represents, there should be significant differences for lead between sampling sites in control and polluted areas. The lead is rapidly washed onto the soil by rain water from the surface also by the death and decomposition of the plant [23,24]. Many literatures have notified the contents of heavy metals were higher in plant samples collected along the roadside of highways [8].

Copper is also one of the major heavy metal considered as an environmental pollutant. Copper is a micronutrient but toxic when it is in excess concentration. The source of copper being due to corrosion of metallic parts of cars derived from engine wear, brushing and bearing metals [25]. The mean Cu level in roadside soil (49.71 µg/gm) found to be much higher than the grass (4.87 µg/gm) and caesalpinia (4.70 µg/gm).

The main source of Zn on the roadside is because of automobile traffic i.e break lining looses of oil and cooling liquid [26]. Arithmetic mean of Zn of the roadside soil from Bagalkot to Mudhol state highway owes relatively high level of 188.31 µg/gm with a range of 32.29 – 381.54 µg/gm. the range of Zn 24.40 – 35.70 µg/gm in caesalpinia and grass 24.50 – 35.8 µg/gm. however, the Zn content in the test plant samples of polluted area are below the allowed limit (15 – 100 µg/gm) [18].

The main sources of environmental cadmium pollution are vehicle wheels, mineral oils increases Cd levels of environment and plants [27]. Cd dispersed in the natural environment through anthropogenic activities as well as natural rock mineralization process and thus, plants can easily absorbs Cd from the soil and also transport to the shoot levels. Cadmium induces complex changes in plants genetical, physiological and biochemical levels. The values were found little higher than allowed limit (1 µg/gm) in plants, i.e the Cd level in roadside soil averaged about 2.0 µg/gm and was observed that Cd was the lowest among the seven metals tested. The mean Cd in caesalpinia was 1.41 µg/gm and in grass, it is found to be 1.57 µg/gm. These findings were in confirmation with Shafia et al. [28].

From the results it was found that the soil, grass and caesalpinia contained high level of Manganese than other limits. Roadside soil, grass and caesalpinia had average 1528.34 µg/gm, 56.606 µg/gm and 56.10 µg/gm respectively. The attribution of Mn content is the lithogenic factor apart from vehicular pollution [29].

Chromium is considered as a serious concern with respect to health of biotics particularly in detrimental to plant growth and development. Cement, limestone industries are the major causes for the high influx of chromium into the atmosphere [29]. Significant differences in our analysis for chromium in soil and in plant samples are found. Chromium level was too high in roadside soil (315.54 µg/gm against control 110.41 µg/gm. In caesalpinia it was found to be 4.61 µg/gm, in grass it is found that 4.90 µg/gm against control (zero). Thus, the Cr content in soil and test plant samples of polluted area are above the maximum allowed limit (soil- 10-200 µg/gm, plant- 0.05-0.5 µg/gm).

Table 2. Metal accumulation profile in caesalpinia, grass and soil

S. no	**Heavy metals**	**Control (µg g-1 dry wt.)**	**Roadside Caesalpinia (µg g-1 dry wt.)**		**Roadside grass (µg g-1 dry wt.)**		**Control (µg g-1 dry wt.)**	**Roadside soil (µg g-1 dry wt.)**	
			Range	**Mean ± SE**	**Range**	**Mean±SE**		**Range**	**Mean± SE**
1	Lead	18.46	20.36-29.39	23.73±1.84	20.16-28.01	23.736±1.84	70.50	81.91-139.8	95.71±8.71
2	Copper	2.15	3.92-5.94	4.70±0.35	3.95-5.76	4.87±0.35	34.91	39.54-58.58	49.71±3.51
3	Zinc	16.19	24.40-35.7	32.84±3.10	24.50-35.8	32.87±3.11	29.84	32.29-381.54	188.3±54.28
4	Cadmium	0.82	1.01-1.78	1.41±0.08	1.15-1.52	1.571±0.082	2.16	1.51-2.08	2.0±0.19
5	Manganese	15.72	27.01-69.10	56.10±7.30	28.91-72.51	56.606±7.36	1254.1	1257.9-2051.5	1528.3±26.5
6	Chromium	N.D	1.20-7.8	4.61±2.20	1.28-8.00	4.90±2.23	110.41	131.9-951.2	315.54±2.46
7	Nickel	6.70	7.9-13.1	9.10±1.40	8.1-15.1	10.51±1.411	69.38	69.53-108.6	85.91±5.91

ND- Not detectable; Mean values ± standard error

Table 3. Correlation coefficient of heavy metals in roadside soil and grass

S. no.	Metal	r. value
1	Lead	0.628*
2	Copper	0.481*
3	Zinc	0.829*
4	Cadmium	0.748*
5	Manganese	0.529*
6	Nickel	0.331*
7	Chromium	0.215*

r= 0.60 and above have significant correlation

Table 4. Correlation coefficient of heavy metals in roadside soil and caesalpinia

S. no.	Metal	r. value
1	Lead	0.627*
2	Copper	0.480*
3	Zinc	0.824*
4	Cadmium	0.740*
5	Manganese	0.520*
6	Nickel	0.321*
7	Chromium	0.210*

r= 0.60 and above have significant correlation

Nickel is a micronutrient required at very low concentration by the plants normally in Ni^{+2} state, at high concentration Ni inhibits plant growth. The maximum Ni content was found 10.5 µg/gm in grass than caesalpinia with 9.10 µg/gm. Generally it is concluded that Ni content in test plant samples of polluted area are higher than the normal values (0.1 – 5.0 µg/gm) in plants [18].

Simple correlations ($r > 0.60$) between the metal Pb, Cu, Ni, Mn, Fe, Zn and Cd were calculated and are given in the Tables 3 and 4. Significant correlations between the metal levels in roadside soil, caesalpinia and grass were found in Zn, Cd and Ni ($r > 0.06$). It may be indicating the bioconcentration of these metals in soil, grass and caesalpinia, in addition to aerial deposition. This may attributed to the favorable root environment [30] i.e soil conditions might have favored their absorption. Correlations in case of chromium, nickel, manganese and copper contents between soil, grass and caesalpinia were low due to low bioavailability of these metals owing to unfavorable root environment. Whatever excess content of these metals found in grass and caesalpinia was presumed to be due to the aerial decomposition contributed by motor vehicles.

Thus, the order of increment of heavy metals in roadside soil is as follows: Mn > Cr > Zn > Pb > Ni > Cu > Cd, whereas in grass: Mn> Zn> Pb> Ni> Cr> Cu> Cd and in caesalpinia: Mn>Zn > Pb> Ni> Cu> Cr > Cd. The elevated levels of heavy metals in the roadside soil, grass and caesalpinia is an evidence of airborne pollutants of roadside environment along the state high way of Bagalkot to Mudhol. Soils due to their cation exchange capacity (CEC), complexing organic substances, oxides and carbonates, have high retention capacity for the heavy metals [31]. Thus, contamination levels increase continuously as long as the nearby sources remain active. During the last decade, the Bagalakot to Mudhol state high way has witnessed sharp increase in vehicle number due to urbanization. Similar observation in Caesalpinia in Madhurai city of southern region of Tamil Nadu [32].

In soil, the lesser mobility of metals and its accumulation on a long-term basis, leads to overall higher contamination level of metals; whereas, in roadside grass, caesalpinia it represents more accumulation due to turnover of plant materials (like new growths, the senescence followed by abscission of old parts) and meteorological influences [33]. Thus, the study of metal concentration of both roadside soil, grass and caesalpinia reflects the extent of aerial contamination of the roadside environment. The penetration of heavy metals into the food chains due to vehicular emissions may cause a long- range ecological and health hazard.

The results of our study indicate that the concentration of heavy metals such as Pb, Cd, Mn, Ni, Cu and Cr from the traffic area is an indicative of anthropogenic pollution.

4. CONCLUSION

It was concluded that with an increase in the amount of heavy metals in soil and their uptake by plants also increase. The mobility of heavy metals are highly translocated from soil to plant leaves in all the sampling sites. According to our study grass shows slight greater accumulation potentiality than caesalpinia. High metal concentrations in plants are contained in urban and highway roadsides due to the anthropogenic activities in addition to the traffic density. The heavy metal concentration was maximum in the study area along the roadside of Bagalkot to Mudhol. Caesalpinia is widely distributed at Bagalkot (Navanagar) is used as roadside ornamental plant and the grass is the good food for grazing animals. In accordance with the data presented here grass and caesalpinia possess all characteristics and are selected as bioindicators.

There is also a need for enforcement of regulations to control environmental pollution. Public participation, non-governmental organization and civic agencies of the government required collective approach towards the solution. Continuous air monitoring for one or more pollutants is an absolute necessity for completing a diagnosis of pollutant level in the air, water and soil environment. Most importantly, a network of monitoring stations throughout the country would be helpful to measure the current pollutant level. Accumulation of air monitoring data will provide the criteria needed for establishing air quality standards.

ACKNOWLEDGEMENT S

The authors are thankful to the Principal, BLDEA's Degree College, Jamkhandi (Karnataka), Principal, JSS College Dharwad and to the Chairman, PG Department Botany, Karnatak University, Dharwad (Karnataka) for providing necessary facilities to carry out research work.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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