Available online www.jocpr.com

Journal of Chemical and Pharmaceutical Research, 2016, 8(3):51-57

Research Article

ISSN : 0975-7384
CODEN(USA) : JCPRC5

The Schultz and modified Schultz polynomials of certain subdivision and line subdivision graphs

Mohammad Reza Farahani[1] and Muhammad Kamran Jamil[2*]

[1]*Department of Applied Mathematics of Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran*
[2]*Abdus Salam School of Mathematical Sciences, Government College University, Lahore, Pakistan*

ABSTRACT

For a connected graph G(V(G),E(G)), d_u and d(u,v) represents the degree of u and the distance between u and v. Ivan Gutman defined the Schultz and modified Schultz polynomials as $Sc(G,x)=\sum_{\{u,v\}\subseteq V(G)}(d_u+d_v)x^{d(u,v)}$ *and* $Sc^*(G,x)=\sum_{\{u,v\}\subseteq V(G)}d_ud_vx^{d(u,v)}$ *, respectively. Such that their first derivative at x=1 are equal to* $Sc(G)=\sum_{\{u,v\}\subseteq V(G)}(d_u+d_v)d(u,v)$ *and* $Sc^*(G)=\sum_{\{u,v\}\subseteq V(G)}(d_ud_v)d(u,v)$ *, respectively, which are the Schultz index and its modification. In this paper, we compute the Schultz and modified Schultz polynomials and their corresponding indices of the subdivision graph and the line graph subdivision graph of wheel graph.*

Keywords: Topological indices, Schultz indices, Schultz polynomial, subdivision graph, line graph.
Mathematics Subject Classification; *05C05, 05C12, 05C15, 05C31, 05C69.*

INTRODUCTION

Let *G(V(G),E(G))* be a simple connected graph, where the *V(G)* and *E(G)* are the vertex and edge sets, respectively, of G. For vertices $u,v\in V(G)$, *u* is adjacent to *v* if they are connected by an edge. The degree of a vertex *u*, d_u, is the number of vertices adjacent to *u*. The distance between *u* and *v*, *d(u,v),* is the number of edges in a shortest path connecting them. The largest distance between any two vertices of a graph *G* is called the *diameter* of *G*, denoted as d(G).

The *subdivision graph* is the graph obtained by inserting an additional vertex into each edge of *G*, denoted as S(G). The *line graph,* of a graph *G* is the graph whose vertices are the edges of the graph *G*, and two vertices *e* and *f* are incident if and only if they are adjacent in *G,* denoted as L(G). A *wheel graph* with *n* vertices is a graph formed by connecting a single vertex to all vertices of a cycle, denoted as W_n. It has *2(n-1)* edges. For further study and results we refer [21-23].
Distance is an important concept in graph theory and it has numerous applications in computer science, biology, chemistry and a variety of other fields. Using the concept of distances in a graph *G*, *H. Wiener* defined a descriptor for explaining the boiling points of paraffins [1]

$$W(G)=\sum_{\{u,v\}\subseteq V(G)}d(u,v)$$

This descriptor is known as Wiener index. A topological index is a real number related to a structural graph of a molecule, and it does not depend on the labelling or pictorial representation of a graph. A lot of topological indices have been introduced, Wiener index is one of the topological indices that correlate with some of the physico-chemical properties of the compound [2,3].

Harry Shultz [5] introduced another distance based topological index known as Shultz index

$$Sc(G) = \sum_{\{u,v\}\subseteq V(G)} (d_u + d_v)d(u,v)$$

The Schultz index is closely related to the Wiener index in the case of trees with relation $S(G) = 4W(G) - n(n-1)$ [6]. *Gutman et. al.* [7] defined the modified Schultz index as

$$Sc^*(G) = \sum_{\{u,v\}\subseteq V(G)} (d_u d_v)d(u,v)$$

This topological index also closely related to Wiener index with relation [8].

$$Sc^*(G) = 4W(G) - n(2n-1)$$

H. Hosoya [4] introduced a distance-based polynomial to generate distance distributions for graphs, called the Wiener polynomial

$$H(G,x) = \sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$$

The first derivative of *H(G,x)* at *x=1* is equal to Wiener index of *G*. Gutman [9] introduced new polynomials called the Schultz polynomial and the modified Schultz polynomial as

$$Sc(G,x) = \sum_{\{u,v\}\subseteq V(G)} (d_u + d_v)x^{d(u,v)}$$

$$Sc^*(G,x) = \sum_{\{u,v\}\subseteq V(G)} d_u d_v x^{d(u,v)}$$

Such that their derivative at x=1 are equal to the Schultz and modified Schultz indices. He also obtained some connection between these polynomials and Wiener polynomial of trees. For further details we refer [10-20].

RESULTS AND DISCUSSION

In this section, we compute the Schultz and modified Schultz polynomials and their corresponding Schultz and modified Schultz topological indices of subdivision graph of the wheel graph $S(W_n)$ and the line graph subdivision graph of the wheel graph $L(S(W_n))$.

Theorem 1. Let $S(W_n)$ be the subdivision graph of the wheel graph with order $n\geq 3$. Then,

- The Schultz polynomial and index of $S(W_n)$ are equal to

$Sc(S(Wn),x)=(n^2+17n)x+(3n^2+19n)x^2+(6n^2+7n)x^3+(4n^2+2n)x^4+(5n^2-20n)x^5+(2n^2-10n)x^6.$

$Sc(S(Wn))=78n^2-76n.$

- The Modified Schultz polynomial and index of $S(W_n)$ are equal to

$Sc^*(S(W_n),x)=(n^2+18n)x+(5n^2+19n)x^2+(8n^2+6n)x^3+(8n^2+5n)x^4+(6n^2-24n)x^5+(2n^2-10n)x^6.$

$Sc^*(S(Wn))=109n^2-86n.$

Proof. Consider the subdivision graph of a wheel graph W_n with order $n\geq 3$. By definitions of the subdivision graph and the wheel graph, one can see that the number of vertices in $S(W_n)$ is equal to $|V(S(W_n))|=|V(W_n)|+|E(W_n)|=3n+1$, in which $2n$ vertices of $S(W_n)$ have degree 2 and n vertices of the subdivision graph of W_n have degree 3 and only center vertex c has degree n.

Thus, we divide the vertex set $V(S(W_n))$ in three partitions

$V_2=\{v\in V(S(W_n))|\ d_v=2\},$

$V_3=\{v\in V(S(W_n))|\ d_v=3\},$

$V_n=\{c\in V(S(W_n))|\ d_c=m\}.$

The definition of the subdivision graph of the wheel graph W_n and from Figure 1, the size of these three vertex sub-sets are $|V_2|=2n$, $|V_3|=n$ and $|V_n|=1$ and the number of edges of $S(W_n)$is equal to

$$|E(S(W_n))|=½[2\times|V_2|+3\times|V_3|+n\times|V_n|]=\frac{2\times2n+3\times n+n\times1}{2}=4n.$$

From Figure 1, we see that there are distances between vertices of the subdivision graph of the wheel graph W_n are up to six and the diameter of $S(W_n)$ is equal to $d(S(W_n))=6$. In other words for every vertices $u,v\in V(S(W_n))$; $\exists d(u,v)\in\{1,2,...,6\}$.

Now, from the structure of the subdivision graph of the wheel graph $S(W_n)$ (see Figure 1), we compute all terms of the Schultz polynomial, Modified Schultz polynomial of $S(W_n)$, based on the number of $d(u,v)$ $\forall v,u\in V(S(Wn))$.

Here consider $d(u,v)$=1 ($\forall v,u\in V(S(W_n))$), so from the edge set $E(S(W_n))$, we see that there are n path with length one or n edges $cv\in E(S(W_n))$ for only vertex $c\in V_n\subset V(S(Wn))$ and a vertex $v\in V_2\subset V(S(Wn))$ that $d_c+d_v=n+2$ and $d_c\times d_v=2n$. For a vertex $u\in V_3\subset V(S(Wn))$, there are 3 path with length one until a vertex $v\in V_2$ or $3n$ edges $uv\in E(S(Wn))$ such that $d_u=3$, $d_v=2$ and alternatively $d_u+d_v=5$ & $d_u\times d_v=6$. Therefore the first terms of the Schultz and Modified Schultz polynomials of $S(Wn)$ will be $n(n+2)x+3n(5)x=(n^2+17n)x$ and $n(2n)x+3n(6)x=(2n^2+18n)x$, respectively.

In case $d(u,v)$=2 $\{v,u\}\subset V(S(W_n))$; there are n 2-edges paths between Center vertex $c\in V_n$ and vertices from $V_3\subset V(S(Wn))$, there are $½(2|V_3|)=n$ 2-edges paths between all vertices $u,v\in V_3$ that $d_u+d_v=6$ & $d_u\times d_v=9$. Finally there are $½[2n+n(n-1)+4n]=½(n^2+5n)$ 2-edges paths between all vertices uv from $V_2\subset V(S(Wn))$, such that $d_u+d_v=d_u\times d_v=4$. Then the second terms of the Schultz and Modified Schultz polynomials of $S(Wn)$ are equal to $[6\times n+(n+3)\times n+4\times½(n^2+5n)]x^2=(3n^2+19n)x^2$ and $[9\times n+(3n)\times n+4\times½(n^2+5n)]x^2=(5n^2+19n)x^2$, respectively.

Here, we can compute all other terms of the Schultz and Modified Schultz polynomials of $S(W_n)$ by using the definition of the subdivision graph of the wheel graph (Figure 1). Thus, we present all coefficients and terms of the Schultz and Modified Schultz polynomials of $S(Wn)$ in Table 1 (for all $d(u,v)\in\{1,2,...,6\}$).

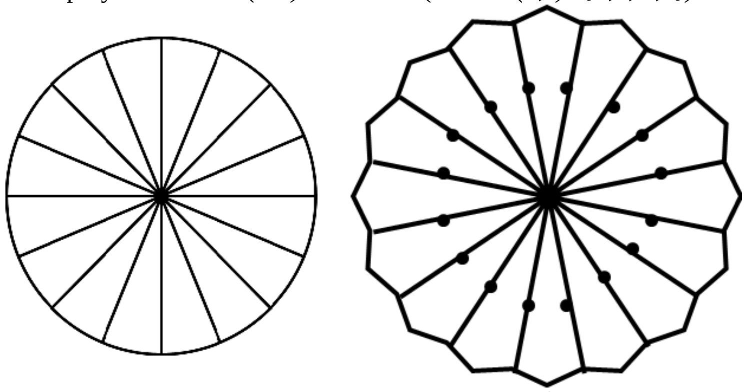

Figure 1. The wheel graph W_{16} and the subdivision graph of a wheel graph W_{16}.

Table 1. all coefficients and terms of the Schultz and Modified Schultz polynomials of $S(Wn)$ $\forall d(u,v)\in\{1,2,...,6\}$ **&** $u,v\in V(S(W_n))$

distance $d(u,v)$	degrees of d_u & d_v	No. $d(u,v)$-edges paths	term of Schultz polynomial $x^{d(u,v)}$	term of Modified Schultz polynomial $x^{d(u,v)}$
1	2 & 2	0	0	0
	2 & 3	$\|V_2\|=3n$	$15n$	$18n$
	3 & 3	0	0	0
	2& n	N	$n(n+2)$	$2n^2$
	3 & n	0	0	0
			n^2+17n	n^2+18n
2	2 & 2	$½(n^2+5n)$	$2(n^2+5n)$	$2(n^2+5n)$
	2 & 3	0	0	0
	3 & 3	N	$6n$	$9n$
	2& n	0	0	0
	3 & n	N	$n(n+3)$	$3n^2$
			$3n^2+19n$	$5n^2+19n$
3	2 & 2	0	0	0
	2 & 3	$\|V_3\|(n-1)+2\|V_3\|$	$5(n^2+n)$	$6(n^2+n)$
	3 & 3	0	0	0
	2& n	$\|V_3\|$	$n(n+2)$	$2n^2$
	3 & n	0	0	0
			$6n^2+7n$	$8n^2+6n$
4	2 & 2	$n(n-2)+n=n^2-n$	$4(n^2-n)$	$4(n^2-n)$
	2 & 3	0	0	0
	3 & 3	n	$6n$	$9n$
	2& n	0	0	0
	3 & n	0	0	0
			$4n^2+2n$	$8n^2+5n$
5	2 & 2	0	0	0
	2 & 3	$\|V_3\|(\|V_3\|-4)$	$5(n^2-4n)$	$6(n^2-4n)$
	3 & 3	0	0	0
	2& n	0	0	0
	3 & n	0	0	0
			$5n^2-20n$	$6n^2-24n$
6	2 & 2	$½n(n-5)$	$2n(n-5)$	$2n(n-5)$
	2 & 3	0	0	0
	3 & 3	0	0	0
	2& n	0	0	0
	3 & n	0	0	0
			$2n^2-10n$	$2n^2-10n$

Now, from Table 1, we see the Schultz, Modified Schultz polynomials of the subdivision graph of the wheel graph *S(Wn)* are equal to:

$$Sc(S(Wn),x)=½\sum_{u,v\in V(S(Wn))}(d_u+d_v)x^{d(u,v)}$$
$$=(n^2+17n)x+(3n^2+19n)x^2+(6n^2+7n)x^3+(4n^2+2n)x^4+(5n^2-20n)x^5+(2n^2-10n)x^6.$$

$$Sc^*(S(W_n),x)=½\sum_{u,v\in V(S(Wn))}(d_u\times d_v)x^{d(u,v)}$$
$$=(n^2+18n)x+(5n^2+19n)x^2+(8n^2+6n)x^3+(8n^2+5n)x^4+(6n^2-24n)x^5+(2n^2-10n)x^6.$$

Also, by definitions of the Schultz, Modified Schultz indices, we have

$$Sc(S(Wn))=\left.\frac{\partial Sc(S(Wn),x)}{\partial x}\right|_{x=1}$$
$$=\frac{\partial}{\partial x}\left((n^2+17n)x+(3n^2+19n)x^2+(6n^2+7n)x^3+(4n^2+2n)x^4+(5n^2-20n)x^5+(2n^2-10n)x^6\right)_{x=1}$$
$$=78n^2-76n.$$

$$Sc^*(S(Wn))=\left.\frac{\partial Sc^*(S(Wn),x)}{\partial x}\right|_{x=1}$$

$$=\frac{\partial}{\partial x}\left((n^2+18n)x+(5n^2+19n)x^2+(8n^2+6n)x^3+(8n^2+5n)x^4+(6n^2-24n)x^5+(2n^2-10n)x^6\right)_{x=1}$$

$$=(n^2+18n)\times 1+(5n^2+19n)\times 2+(8n^2+6n)\times 3+(8n^2+5n)\times 4+(6n^2-24n)\times 5+(2n^2-10n)\times 6$$
$$=109n^2-86n.$$

Thus, this completed the proof of Theorem 1. ■

Theorem 2. Let $L(S(W_n))$ be the line graph of the subdivision graph of the wheel graph. Then,

- The Schultz polynomial and index of $L(S(W_n))$ are equal to

$Sc(L(S(W_n)),x)=(2n^3+27n)x+(n^3+4n^2+27n)x^2+(2n^3+7n^2+15n)x^3+(12n^2-24n)x^4+(6n^2-54n)x^5$
$Sc(L(S(W_n)))=10n^3+107n^2-240n.$

- The Modified Schultz polynomial and index of $L(S(W_n))$ are equal to

$Sc^*(L(S(W_n)),x)=(½n^4-½n^3+3n^2+36n)x+(3n^3+3n^2+36n)x^2+½(12n^3-3n^2+63n)x^3+(18n^2-36n)x^4+(9n^2-81n)x^5$
$Sc^*(L(S(W_n)))=½n^4+7n^3+{}^{243}\!/_{2}\,n^2-252n.$

Proof. Consider $L(S(W_n))$ as the line graph of the subdivision graph of the wheel graph "W_n" with order $\forall n\geq 3$. From the definitions of subdivision and line graphs in Section 1, we see that a general form of $L(S(W_n))$ $|V(L(S(W_n)))|=4n$ vertices and $|E(L(S(W_n)))|=½n(n+9)$ edges. Also, from Figure 2, we see that $L(S(W_n))$ has n vertices with degree n and 3n vertices with degree 3. In other words, we have two sub-sets of $V(L(S(W_n)))$ as follow:

$V_n=\{v\in V(L(S(W_n)))|\ d_v=n\}$
$V_3=\{v\in V(L(S(W_n)))|d_v=3\}$

Such that $V(L(S(W_n)))=V_n\cup V_3$ & $|V_n|=n$ and $|V_3|=3n$ $(|E(L(S(W_n)))|=½(3|V_3|+n|V_n|)=½n(n+9)$.

Here from Figure 2, one can see that the diameter of $L(S(W_n))$ is equal to five (the diameter $d(G)$ of G is the longest topological distance between vertices in $V(G)$.). Obviously $\forall u,v\in V(L(S(W_n)))$; $d(u,v)$ is equal to $1,2,...,5$.

Now, similar to proof of Theorem 1, we compute all terms of the Schultz polynomial, Modified Schultz polynomial of the line graph of the subdivision graph of the wheel graph by using the number of $d(u,v)$ for all pairs of $u,v\in V(L(S(W_n)))$. Thus, we present all cases $d(u,v)\in\{1,2,...,5\}$ $\forall\{v,u\}\subset V(L(S(W_n)))$ of $L(S(W_n))$ in Table 1 by using the definitions of subdivision and line graphs and the general representation of $L(S(W_n))$ in Figure 2.

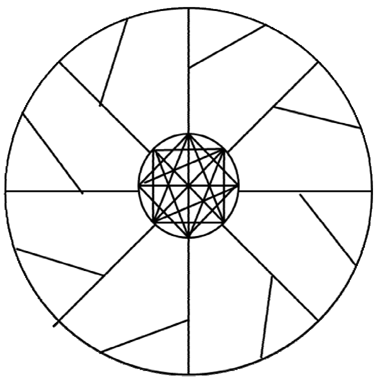

Figure 2. The line graph of the subdivision graph of the wheel graph W_8

Table 2. All coefficients and terms of the Schultz and Modified Schultz polynomials of $L(S(W_n))$ $\forall d(u,v)=1,2,...,5$

distance $d(u,v)$	degrees of d_u & d_v	No. $d(u,v)$-edges paths	term of Schultz polynomial $x^{d(u,v)}$	term of Modified Schultz polynomial $x^{d(u,v)}$
1	3 & 3	$4n$	$24n$	$36n$
	3 & n	n	n^2+3n	$3n^2$
	n & n	$\|E(K_n)\|=½(n^2-n)$	n^3-n^2	$½n^4-½n^3$
			$2n^3+27n$	$½n^4-½n^3+3n^2+36n$
2	3 & 3	$4n$	$24n$	$36n$
	3 & n	n^2+n	n^3+4n^2+3n	$3n^3+3n^2$
	n & n	0	0	0
			n^3+4n^2+27n	$3n^3+3n^2+36n$
3	3 & 3	$2n+½n(n-1)+2n$ $=½n(n+7)$	$3n^2+21n$	$\frac{9}{2}n^2+\frac{63}{2}n$
	3 & n	$2n(n-1)$	$2n^3+4n^2-6n$	$6n^3-6n^2$
	n & n	0	0	0
			$2n^3+7n^2+15n$	$6n^3-\frac{3}{2}n^2+\frac{63}{2}n$
4	3 & 3	$n(n-2)+n(n-2)$	$12n^2-24n$	$18n^2-36n$
	3 & n	0	0	0
	n & n	0	0	0
			$12n^2-24n$	$18n^2-36n$
5	3 & 3	$½[2n(n-9)]$	$6n^2-54n$	$9n^2-81n$
	3 & n	0	0	0
	n & n	0	0	0
			$6n^2-54n$	$9n^2-81n$

For example, 1n case $d(u,v)$=1, we know that all 1-edge-paths of $L(S(W_n))$ are all edges of $L(S(W_n))$, clearly. And all edges of the line graph $S(W_n)$ are the 2-edge-paths of $S(W_n)$. So by according to the proof of Theorem 1, we can conclude the first terms of the Schultz and Modified Schultz polynomials of $L(S(W_n))$ of the second terms of the Schultz and Modified Schultz polynomials of $S(Wn)$ as follow:

$$[6\times4n+(n+3)\times n+(n+n)\times½(n^2-n)\ ]x^2=(2n^3+27n)x^1$$

and

$$[9\times4n+(3n)\times n+(n^2)\times½(n^2-n)]x^2=(½n^4-½n^3+3n^2+36n)x^1$$

In case $d(u,v)$=2 $\{v,u\}\subset V(L(S(W_n)))$; there are n^2+n 2-edges paths between vertices of the vertex partition V_n and V_3, such that $d_u+d_v=n+3$ & $d_u\times d_v=3n$. Also, $n+n+2n$ 2-edges paths between all vertices of V_3, that $d_u+d_v=6$ & $d_u\times d_v=9$. And these imply that the second terms of the Schultz and Modified Schultz polynomials of $L(S(W_n))$ be $[6\times4n+(n+3)\times(n^2+n)]x^2=(n^3+4n^2+27n)x^2$ and $[9\times4n+(3n)\times(n^2+n)]x^2=(3n^3+3n^2+36n)x^2$, respectively.

Now, we present the coefficients and other terms of the Schultz and Modified Schultz polynomials of $L(S(W_n))$ in Table 2. Thus, by using the results from above mentions and Table 2, we can compute $Sc(L(S(W_n)),x)$ and $Sc^*(L(S(W_n)),x)$ as follow:

$$Sc(L(S(W_n)),x)=(2n^3+27n)x+(n^3+4n^2+27n)x^2+(2n^3+7n^2+15n)x^3+(12n^2-24n)x^4+(6n^2-54n)x^5$$

$$Sc^*(L(S(W_n)),x)=(½n^4-½n^3+3n^2+36n)x+(3n^3+3n^2+36n)x^2+½(12n^3-3n^2+63n)x^3+(18n^2-36n)x^4+(9n^2-81n)x^5$$

Finally, the Schultz and Modified Schultz indices of the line graph of the subdivision graph of the wheel graph $L(S(W_n))$ are equal to

$$Sc(L(S(W_n)))=\left.\frac{\partial Sc(L(S(W_n)),x)}{\partial x}\right|_{x=1}=10n^3+107n^2-240n,$$

$$Sc^*(L(S(W_n)))=\left.\frac{\partial Sc^*(L(S(W_n)),x)}{\partial x}\right|_{x=1}=\tfrac{1}{2}n^4+7n^3+\tfrac{243}{2}n^2-252n.$$

Here, the proof of Theorem 2 was completed. ■

REFERENCES

[1] H. Wiener, *J. Am. Chem. Soc.*, 69 (**1947**) 17-20.
[2] A. A. Dobrynin, R. Entringer, I Gutman, *Acta Appl. Math*., 66 (**2001**) 211-249.
[3] I. Gutman, O. E. Polansky: *Mathematical concepts in organic chemistry*, Springer, Berlin, **1986**.
[4] H. Hosoya, *Discrete Appl. Math*., 19 (**1988**) 239-257.
[5] H. P. Schultz, *J. Chem. Inf. Comput. Sci*. 29 (**1989**) 227-228.
[6] D. J. Klein, Z. Mihalić, D. Plavšić, N. Trinjastić, *J. Chem. Inf. Comput. Sci.*, 32 (**1992**) 304-305.
[7] I. Gutman, S. Klavzar, *Disc. Appl. Math.*, 80 (**1997**) 73-81.
[8] I. Gutman, J. *Chem. Inf. Comput. Sci*., 34 (**1994**) 1087-1089.
[9] I. Gutman, *Sciences mathematiques*, 30 (**2005**) 1-7.
[10] M. Eliasi, B. Taeri, *Appl. Anal. Discrete Math*. 2 (**2008**) 285-296.
[11] F. Hassani, A. Iranmanesh, S. Mirzaie, *MATCH Commun. Math. Comput. Chem.* 69 (**2013**) 87-92.
[12] M.R. Farahani, M.P. Vlad. On the Schultz, *Studia UBB Chemia*. 57(4), (**2012**), 55-63.
[13] M.R. Farahani, M.P. Vlad. On the Schultz, *Studia UBB Chemia.* 57(4), (**2012**), 55-63.
[14] M.R. Farahani. Hosoya, Schultz, *International Journal of Theoretical Chemistry.* 1(2), (**2013**), 09-16.
[15] M.R. Farahani. *Int. J. Applications of Discrete Mathematics.* 1(1), (**2013**), 1-8.
[16] M.R. Farahani. *J. Applied Math. & Info.* 31(5-6), (**2013**). 595-608.
[17] M.R. Farahani. *Pacific Journal of Applied Mathematics.* 6(3), (**2014**), 77-84.
[18] M.R. Farahani, Wei Gao & M.R. Rajesh Kanna. *Asian Journal of Applied Sciences.* **2015**, 3(6), 823-827.
[19] M.R. Farahani, Wei Gao. *Applied Mathematics.* 6, **2015**, 2319-2325.
[20] M.R. Farahani, M.R. Rajesh Kanna and Wei Gao.. *Journal of Chemical, Biological and physical sciences* 6(1), **2016**, 294-301.
[21] G. Su, L. Xu, *Applied Mathematics and Computation* 253 (**2015**) 395-401.
[22] M. F. Nadeem, S. Zafar, Z. Zahid, *Applied Mathematics and Computation* 271 (**2015**) 790-794.
[23] M. F. Nadeem, S. Zafar, Z. Zahid, *Applied Mathematics and Computation* 273 (**2016**) 125-130.