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ON THE VERTEX DEGREE POLYNOMIAL OF GRAPHS

H. AHMED[1*], A. ALWARDI[2], R. SALESTINA M.[1], §

Abstract. A novel graph polynomial, termed as vertex degree polynomial, has been conceptualized, and its discriminating power has been investigated regarding its coefficients and the coefficients of its derivatives and their relations with the physical and chemical properties of molecules. Correlation coefficients ranging from 95% to 98% were obtained using the coefficients of the first and second derivatives of this new polynomial. We also show the relations between this new graph polynomial, and two oldest Zagreb indices, namely the first and second Zagreb indices. We calculate the vertex degree polynomial along with its roots for some important families of graphs like tadpole graph, windmill graph, firefly graph, Sierpinski sieve graph and Kragujevac trees. Finally, we use the vertex degree polynomial to calculate the first and second Zagreb indices for the Dyck-56 network and also for the chemical compound triangular benzenoid $G[r]$.

Keywords: Vertex degree polynomial, Vertex degree roots, First Zagreb index, Second Zagreb index, Kragujevac tree.

AMS Subject Classification: 05C07, 05C31, 05C35.

1. Introduction

In this paper, all graphs are assumed to be simple and finite without isolated vertices. A graph $G = (V, E)$ is a nonempty set of objects called vertices together with a set of pairs of distinct vertices of G called edges. The vertex set and the edge set of G are denoted by $V(G)$ and $E(G)$ respectively. The edge $e = \{u, v\}$ is said to join the vertices u and v. We write $e = uv$ and say that u and v are adjacent vertices, u and e are incident, as are v and e. A vertex u is called a neighbor of v in G if uv is an edge of G. The set $N(v)$ of all neighbors of v is called the open neighborhood of v. Thus $N(v) = \{u \in V : uv \in E\}$. The closed neighborhood of v in G is defined as $N[v] = N(v) \cup \{v\}$. The degree of a vertex v in a graph G is defined to be the number of edges incident with v and is denoted by $d_G(v)$ or $d(v)$. In other words $d(v) = |N(v)|$. A graph G is connected if for every two vertices $u, v \in V$, there exists a (u, v)-path in G. Otherwise, G is said to be

[1] Department of Mathematics Yuvaraja's college, University of Mysore, Mysuru, India.
e-mail: hananahmed1a@gmail.com; ORCID: https://orcid.org/0000-0002-4008-4873.
[*] Corresponding author.
e-mail: ruby.salestina@gmail.com; ORCID: https://orcid.org/0000-0002-3318-2061.
[2] Department of Mathematics, Faculty of Science, University of Jeddah, Jeddah, Saudi Arabia.
e-mail: a-wardi@hotmail.com; ORCID: https://orcid.org/0000-0002-1908-6006.
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disconnected. For more detailed information about the fundamental topics on graphs, see [1, 2, 3, 4, 5, 6, 7, 14, 15, 16]. One of the oldest descriptors of molecular structure is the Zagreb indices, as their properties have been extensively verified and have attracted the attention and interest of researchers in mathematical chemistry. These indices were defined in 1970s [10, 11]. The first and second Zagreb indices were defined as follows

$$M_1(G) = \sum_{v \in V(G)} d^2(v) = \sum_{uv \in E(G)} d(u) + d(v),$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

For properties of these indices see [8, 12, 13].

2. The Motivation

Graph polynomials are helpful in measuring the structural information of networks using combinatorial graph invariants. Also, the graph polynomials are used for the characterization of graphs. Using graph polynomials, many problems in graph theory and discrete mathematics can be solved efficiently. These polynomials have been found very useful in disciplines related to engineering, information science, mathematical chemistry, etc. A graph polynomial is used to represent a graph in an algebraic form. Also, topological indices are based on the degree of vertices. These two factors have motivated us to define a new graph polynomial which is used to calculate the first and second Zagreb indices and we call this polynomial as vertex degree polynomial denoted as $VD(G, x)$. In this paper, the significant result, we have obtained is that the derivative of $VD(G, x)$ at $x = 1$ is two times the second Zagreb index $M_2(G)$ and the sum of coefficients of the vertex degree polynomial is equal to first Zagreb index $M_1(G)$. This result opens a new gateway to the study of the first and second Zagreb indices and their implications. We have also studied using the vertex degree polynomial to model physicochemical properties such as entropy (S), enthalpy of vaporization (HVAP), acentric factor (AcentFac), and standard enthalpy of vaporization (DHVAP) of octane isomers. The values of the physical and chemical properties of octane isomers (Table 1), are taken from www.moleculardescriptors.eu. In Table 2, we calculate the vertex degree polynomial and its derivatives at $x = 1$ for the chemical graphs of octane isomers. Table 3, shows that $D_x(VD(G, x))|_{x=1}$ is strongly correlated with the acentric factor ($|r| = 0.9864$) and entropy (S) ($|r| = 0.9417$), (see Fig 1). Also, $D_x(VD(G, x))|_{x=1}$ is correlated with enthalpy of vaporization (HVAP) ($|r| = 0.7281$) and standard enthalpy of vaporization (DHVAP) ($|r| = 0.8118$), (see Fig 2). Also Table 3, shows that $(VD(G, x))|_{x=1}$ is strongly correlated with the acentric factor ($|r| = 0.9731$) and entropy (S) ($|r| = 0.9543$).And $(VD(G, x))|_{x=1}$ is correlated with (HVAP) ($|r| = 0.886$) and (DHVAP) ($|r| = 0.9361$). Table 3, shows that $D_x^2(VD(G, x))|_{x=1}$ is strongly correlated with the acentric factor ($|r| = 0.9798$) and entropy (S) ($|r| = 0.9522$), (see Fig 3). $D_x^2(VD(G, x))|_{x=1}$ is correlated with enthalpy of vaporization (HVAP) ($|r| = 0.717$) and standard enthalpy of vaporization (DHVAP) ($|r| = 0.8031$), (see Fig 4).

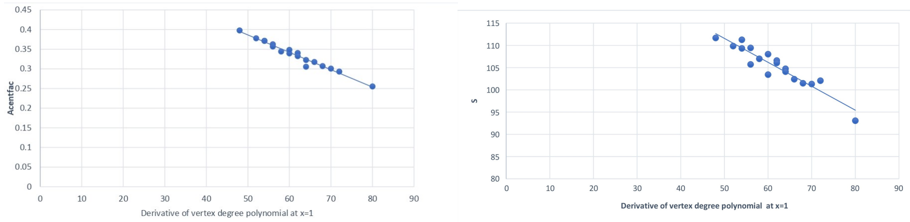

FIGURE 1. Scatter plot of $D_x(VD(G,x))|_{x=1}$ and (a)AcentFac (b) entropy.

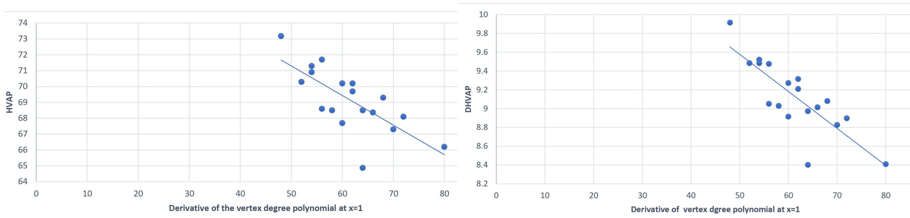

FIGURE 2. Scatter plot of $D_x(VD(G,x))|_{x=1}$ and (a)HVAP (b) DHVAP.

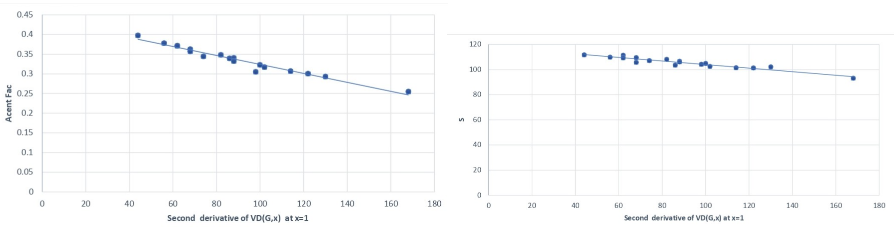

FIGURE 3. Scatter plot of $D_x^2(VD(G,x))|_{x=1}$ and (a)AcentFac (b) entropy.

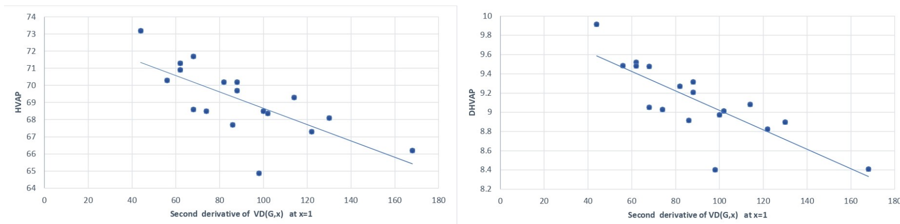

FIGURE 4. Scatter plot of $D_x^2(VD(G,x))|_{x=1}$ and (a)HVAP (b) DHVAP.

3. The Vertex degree polynomial of graphs

Definition 3.1. *Let $G = (V, E)$ be a simple graph without isolated vertex, the vertex degree polynomial of a graph G is defined as*

$$VD(G,x) = \sum_{uv \in E(G)} d(u)x^{d(v)},$$

where the summation is around both possibilities $uv \in E(G)$ and $vu \in E(G)$. The roots of the vertex degree polynomial are called vertex degree roots.
The set of vertex degree roots of the vertex degree polynomial of graph G is denoted by $Z_{VD}(VD(G,x))$.

	Octanes	Acent Fac.	S	HVAP	DHVAP
1	n-octane	0.397898	111.67	73.19	9.915
2	2-methyl heptane	0.377916	109.84	70.3	9.484
3	3-methyl heptane	0.371002	111.26	71.3	9.521
4	4-methyl heptane	0.371504	109.32	70.91	9.483
5	3-ethyl hexane	0.362472	109.43	71.7	9.476
6	2,2-dimethyl hexane	0.339426	103.42	67.7	8.915
7	2,3-dimethyl hexane	0.348247	108.02	70.2	9.272
8	2,4-dimethyl hexane	0.344223	106.98	68.5	9.029
9	2,5-dimethyl hexane	0.356830	105.72	68.6	9.051
10	3,3-dimethyl hexane	0.322596	104.74	68.5	8.973
11	3,4-dimethyl hexane	0.340345	106.59	70.2	9.316
12	2-methyl-3-ethyl pentane	0.332433	106.06	69.7	9.209
13	3-methyl-3-ethyl pentane	0.306899	101.48	69.3	9.081
14	2,2,3-trimethyl pentane	0.300816	101.31	67.3	8.826
15	2,2,4-trimethyl pentane	0.30537	104.09	64.87	8.402
16	2,3,3-trimethyl pentane	0.293177	102.06	68.1	8.897
17	2,3,4-trimethyl pentane	0.317422	102.39	68.37	9.014
18	2,2,3,3-tetramethyl butane	0.255294	93.06	66.2	8.41

TABLE 1. Some physicochemical properties of octane isomers.

Octanes	$VD(G,x)$	$D_x(VD(G,x))\|_{x=1}$	$VD(G,x)\|_{x=1}$	$D_x^2(VD(G,x))\|_{x=1}$
1	$22x^2+4x$	48	26	44
2	$4x^3+16x^2+8x$	52	28	56
3	$5x^3+16x^2+7x$	54	28	62
4	$5x^3+16x^2+7x$	54	28	62
5	$6x^3+16x^2+6x$	56	28	68
6	$5x^4+13x^2+14x$	60	32	86
7	$11x^3+8x^2+11x$	60	30	82
8	$9x^3+10x^2+11x$	58	30	74
9	$8x^3+10x^2+12x$	56	30	68
10	$6x^4+14x^2+12x$	64	32	100
11	$12x^3+8x^2+10x$	62	30	88
12	$12x^3+8x^2+10x$	62	30	88
13	$7x^4+15x^2+10x$	68	32	114
14	$6x^4+7x^3+4x^2+17x$	70	34	122
15	$5x^4+4x^3+7x^2+18x$	64	34	98
16	$7x^4+6x^3+5x^2+16x$	72	34	130
17	$17x^3+15x$	66	32	102
18	$14x^4+24x$	80	38	168

TABLE 2. Vertex degree polynomials of octane isomers and its derivatives at $x=1$.

$\lvert r\rvert$	Acent Fac.	S	HVAP	DHVAP
$VD(G,x)\vert_{x=1}$	0.9731	0.9543	0.886	0.9361
$D_x(VD(G,x))\vert_{x=1}$	0.9864	0.9417	0.7281	0.8118
$D_x^2(VD(G,x))\vert_{x=1}$	0.9798	0.9522	0.717	0.8031

TABLE 3. The correlation coefficient of $VD(G,x)|_{x=1}$, $D_x(VD(G,x))|_{x=1}$ and $D_x^2(VD(G,x))|_{x=1}$ with acentric factor (AcentFac), entropy (S), enthalpy of vaporization (HVAP), and standard enthalpy of vaporization (DHVAP).

Example 3.1. *Let G be a graph in Fig 5.*

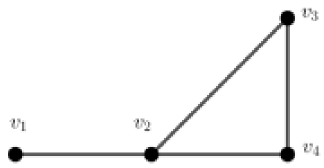

FIGURE 5. The Graph G

$$\begin{aligned} VD(G,x) &= \sum_{uv\in E(G)} d(u)x^{d(v)} \\ &= d(v_1)x^{d(v_2)} + d(v_2)x^{d(v_1)} + d(v_2)x^{d(v_3)} + d(v_3)x^{d(v_2)} \\ &+ d(v_3)x^{d(v_4)} + d(v_4)x^{d(v_3)} + d(v_2)x^{d(v_4)} + d(v_4)x^{d(v_2)} \\ &= 5x^3 + 10x^2 + 3x. \end{aligned}$$

Hence, the set of vertex degree roots is

$$Z_{VD}(G) = \{0, -1 + \frac{1}{5}\sqrt{10}, -1 - \frac{1}{5}\sqrt{10}\}.$$

Theorem 3.1. *Let G be a graph with vertex degree polynomial $VD(G,x)$. Then*

$$D_x(VD(G,x))|_{x=1} = 2M_2(G),$$
$$VD(G,x)|_{x=1} = M_1(G).$$

Proposition 3.1. (1) *For any positive integers n, k such that nk is even and $k \leq n-1$, $VD(G,x) = nk^2x^k$ if and only if G is a $k-$regular connected graph of $n-$vertices.*

(2) *For any path P_n, $VD(P_n,x) = 4x + (4n-10)x^2$. Further, $Z_{VD}(VD(P_n,x)) = \{0, \frac{-2}{2n-5}\}$.*

(3) *Let G be the complete bipartite graph $K_{r,s}$ with $r < s$. Then $VD(G,x) = s^2rx^r + r^2sx^s$. Further, $Z_{VD}(VD(G,x)) = \{0, \sqrt[s-r]{\frac{-s}{r}}\}$.*

(4) *For any wheel graph $G \cong W_n$ with $n \geq 5$ vertices,*
$VD(W_n, x) = (n^2+4n-5)x^3+(3n-3)x^{n-1}$, $Z_{VD}(VD(W_n, x)) = \{0, \sqrt[n-4]{\frac{5-n^2-4n}{3n-3}}\}$.

Corollary 3.1.

(1) $VD(G, x) = n(n-1)^2x^{n-1}$ *if and only if G is the complete graph K_n.*
(2) $VD(G, x) = 4nx^2$ *if and only if G be the cycle graph C_n.*
(3) *If G is the star graph $K_{1,s}$, then* $VD(K_{1,s}, x) = s^2x + sx^s$.
Further, $Z_{VD}(VD(K_{1,s}, x)) = \{0, \sqrt[s-1]{-s}\}$.

Observation 3.1. $Z_{VD}(VD(G, x)) = \{0\}$, *if and only if the graph G is a $k-$regular graph.*

Theorem 3.2. *Let $G_1, G_2, ..., G_m$ be components of G. Then the vertex degree polynomial of G is given as*

$$VD(G, x) = VD(G_1, x) + VD(G_2, x) + ... + VD(G_m, x).$$

Proof. Let $G_1, G_2, ..., G_m$ be components of G. Then $G = \bigcup_{i=1}^{m} G_i$. Note that if $v \in G_i,\ u \in G_j$ for $i \neq j \Rightarrow uv \notin E(G)$ and $uv \in E(G) \Leftrightarrow uv$ belongs to the same component. Hence,

$$\begin{aligned} VD(G, x) &= VD(\bigcup_{i=1}^{m} G_i, x) \\ &= \sum_{u_{1i}v_{1i} \in E(G_1)} d(u_{1i})x^{d(v_{1i})} + ... + \sum_{u_{mi}v_{mi} \in E(G_m)} d(u_{mi})x^{d(v_{mi})} \\ &= VD(G_1, x) + ... + VD(G_m, x). \end{aligned}$$

□

The tadpole graph $T_{r,s}$ is the graph created by joining a cycle graph C_r to a path graph P_s with a bridge.

Theorem 3.3. *For any tadpole graph $T_{r,s}$*

$$VD(T_{r,s}, x) = \begin{cases} 5x^3 + (4r-2)x^2 + 3x, & \text{if } s = 1; \\ 6x^3 + (4s+4r-6)x^2 + 2x, & \text{if } s \geq 2. \end{cases}$$

Further,

$$Z_{VD}(VD(T_{r,s}, x)) = \begin{cases} \{0, \frac{-(4r-2) \pm \sqrt{(4r-2)^2-60}}{10}\}, & \text{if } s = 1; \\ \{0, \frac{-(4s+4r-6) \pm \sqrt{(4s+4r-6)^2-48}}{12}\}, & \text{if } s \geq 2. \end{cases}$$

Proof. <u>**Case (1)**</u> For $s = 1$ and $r \geq 3$, it is clear that the difference between any two consecutive terms $VD(T_{r,1}, x)$, and $VD(T_{r+1,1}, x)$ is $4x^2$......(∗)
In this case the proof is by induction on r.

(1) For $r = 3$ the result is true.
(2) Assume that the result is true for $r = k$ i.e, $VD(T_{k,1}, x) = 5x^3 + (4k-2)x^2 + 3x$.
(3) For $r = k + 1$, we have

$$\begin{aligned} VD(T_{k+1,1}, x) &= 5x^3 + (4(k+1) - 2)x^2 + 3x \\ &= 5x^3 + (4k-2)x^2 + 3x + 4x^2 \\ &= VD(T_{k,1}, x) + 4x^2 \end{aligned}$$

and the result is true by $(*)$.

Case (2) For a given $r \geq 3$, and any $s \geq 2$, it is clear that the difference between any two consecutive terms $VD(T_{r,s}, x)$ and $VD(T_{r,s+1}, x)$ is $4x^2$......$(**)$

In this case the proof is by induction on s.

(1) The result is true for $s = 2$.

(2) Assume that the result is true for $s = k$ i.e, $VD(T_{r,k}, x) = 6x^3 + (4k+4r-6)x^2 + 2x$.

(3) For $s = k+1$

$$\begin{aligned} VD(T_{r,k+1}, x) &= 6x^3 + (4(k+1) + 4r - 6)x^2 + 2x \\ &= 6x^3 + (4k + 4r - 6)x^2 + 2x + 4x^2 \\ &= VD(T_{r,k}, x) + 4x^2 \end{aligned}$$

the result is true by $(**)$.

By solving the equations $VD(T_{r,s}, x) = \begin{cases} 5x^3 + (4r-2)x^2 + 3x, & \text{if } s = 1; \\ 6x^3 + (4s + 4r - 6)x^2 + 2x, & \text{if } s \geq 2. \end{cases}$

we get,

$$Z_{VD}(T_{r,s}) = \begin{cases} \{0, \frac{-(4r-2) \pm \sqrt{(4r-2)^2 - 60}}{10}\}, & \text{if } s = 1; \\ \{0, \frac{-(4s+4r-6) \pm \sqrt{(4s+4r-6)^2 - 48}}{12}\}, & \text{if } s \geq 2. \end{cases}$$ □

The windmill graph is the graph obtained by taking s copies of the complete graph K_n with a vertex in common. It is denoted by $Wd(n, s)$ and consists of s copies of K_n.

Theorem 3.4. *The vertex degree polynomial of windmill graph $Wd(n, s)$ is given by*

$$VD(Wd(n, s), x) = [ns(ns + n^2 - 4n - 2s + 5) + s(s-2)]x^{n-1} + s(n-1)^2 x^{s(n-1)}.$$

Further, $Z_{VD}(VD(Wd(n, s), x)) = \{0, (\frac{-ns(ns+n^2-4n-2s+5)+s(s-2)}{s(n-1)})^{\frac{1}{(s-1)(n-1)}}\}$.

Proof. Let E_1 be the set of all edges which is incident with the center vertex, and E_2 be the set of edges in K_{n-1}. Then

$$\begin{aligned} VD(Wd(n, s), x) &= \sum_{uv \in E(Wd(n,s))} d(u)x^{d(v)} \\ &= \sum_{uv \in E_1} s(n-1)x^{n-1} + (n-1)x^{s(n-1)} + \sum_{uv \in E_2} 2(n-1)x^{n-1} \\ &= s^2(n-1)^2 x^{n-1} + s(n-1)^2 x^{s(n-1)} + s(n-1)^2(n-2)x^{n-1} \\ &= [ns(ns + n^2 - 4n - 2s + 5) + s(s-2)]x^{n-1} + s(n-1)^2 x^{s(n-1)}. \end{aligned}$$

By solving the equation $[ns(ns + n^2 - 4n - 2s + 5) + s(s-2)]x^{n-1} + s(n-1)^2 x^{s(n-1)} = 0$, we get

$Z_{VD}(VD(Wd(n, s), x)) = \{0, (\frac{-ns(ns+n^2-4n-2s+5)+s(s-2)}{s(n-1)})^{\frac{1}{(s-1)(n-1)}}\}$. □

Corollary 3.2. *Let $Wd(3, s)$ be the dutch windmill or n-fan. Then* $VD(Wd(3, s), x) = [3s(s+2) + s(s-2)]x^2 + 4sx^{2s}$.

Further, $Z_{VD}(VD(Wd(3, s), x)) = \{0, (\frac{-3s(S+2)-s(s-2)}{4s})^{\frac{1}{2s-2}}\}$.

A firefly graph $F_{r,s,t}$ is a graph which consists of r triangles, t pendant paths of length 2 and s pendant edges, sharing a common vertex.

Theorem 3.5. $VD(F_{r,s,t}, x) = (4r + 2t + s)x^{2r+t+s} + (4r^2 + t^2 + 4tr + 2sr + st + t + 4r)x^2 + (2t + 2rs + ts + s^2)x$.

Proof. Let E_1 be the set of all edges which are incident with the center vertex, $|E_1| = 2r+t+s$. Let E_2 be the set of all edges uv such that one vertex of degree two and other vertex of degree one, $|E_2| = t$. Let E_3 be the set of all edges which are incident with pendant vertex, $|E_3| = s$. Let E_4 be the set of all edges uv such that u and v of degree two, $|E_4| = r$.

$$
\begin{aligned}
VD(F_{r,s,t},x) &= \sum_{uv\in E(F_{r,s,t})} d(u)x^{d(v)} \\
&= \sum_{uv\in(E_1-E_3)} (2x^{|E_1|} + |E_1|x^2) + \sum_{uv\in E_2}(2x+x^2) + \sum_{uv\in E_3}(|E_1|x + x^{|E_1|}) + \sum_{uv\in E_4}(2x^2+2x^2) \\
&= (2x^{|E_1|} + |E_1|x^2)(|E_1|-s) + t(2x+x^2) + s(|E_1|x + x^{|E_1|}) + 4rx^2 \\
&= (2x^{2r+t+s} + (2r+t+s)x^2)((2r+t+s)-s) + t(2x+x^2) \\
&+ s((2r+t+s)x + x^{2r+t+s}) + 4rx^2 \\
&= (4r+2t+s)x^{2r+t+s} + (4r^2+t^2+4tr+2sr+st+t+4r)x^2 + (2t+2rs+ts+s^2)x.
\end{aligned}
$$

□

Definition 3.2. *Let P_3 be the 3−vertex tree, rooted at one of its terminal vertices. For $k = 2,3,4,...$ 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* [9].

Definition 3.3. *Let $d \geq 2$ be an integer. Let $\beta_1, \beta_2, ..., \beta_d$ specified in Definition 3.2, i.e. $\beta_1, \beta_2, ..., \beta_d \in \{B_2, B_3, ...\}$. A Kragujevac tree T 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, whereas d is the degree of T. The subgraphs $\beta_1, \beta_2, ..., \beta_d$ are the branches of T. Recall that some (or all) branches of T may be mutually isomorphic* [9].

The branch B_k has $2k+1$ vertices. Therefore, if in the Kragujevac tree T, specified in Definition 3.3, $\beta_i \cong B_{ki}$, $i = 1,2,...,d$ then its order is $n(T) = 1 + \sum_{i=1}^{d}(2ki+1)$.

Theorem 3.6. *Let T be the Kragujevac tree, and $s,r,t,...,k,i,j,...,h$ be an integers. Then*

(1) *If $\beta_1 = \beta_2 = ... = \beta_d = B_k$, we have*

$$VD(T,x) = d(k+1)x^d + (d^2 + 2k|B_k|)x^{k+1} + k(k+2)|B_k|x^2 + 2k|B_k|x.$$

(2) *If $\beta_1 \cong B_s$, $\beta_2 \cong B_r$,..., $\beta_d \cong B_k$, and $|B_s| = |B_r| = ... = |B_k| = 1$, we have*

$$
\begin{aligned}
VD(T,x) &= (dx^{s+1} + (s+1)x^d) + (dx^{r+1} + (r+1)x^d) + ... + (dx^{k+1} + (k+1)x^d) \\
&+ s((s+1)x^2 + 2x^{s+1}) + r((r+1)x^2 + 2x^{r+1}) + ... + (s+r+...+k)(x^2+2x).
\end{aligned}
$$

(3) *If $\beta_1 \cong B_s$, $\beta_2 \cong B_r$,...,, $\beta_{d-1} \cong B_z$, $\beta_d \cong B_k$, and $|B_s| = i$, $|B_r| = j$,..., $|B_z| = g$, $|B_k| = h$, we have*

$$
\begin{aligned}
VD(T,x) &= i(dx^{s+1} + (s+1)x^d) + j(dx^{r+1} + (r+1)x^d) + ... + h(dx^{k+1} + (k+1)x^d) \\
&+ s|B_s|((s+1)x^2 + 2x^{s+1}) + r|B_r|((r+1)x^2 + 2x^{r+1}) + ... + k|B_k|((k+1)x^2 + 2x^{k+1}) \\
&+ [s|B_s| + r|B_r| + ... + k|B_k|](x^2+2x).
\end{aligned}
$$

Proof. **Case** (1) If $\beta_1 = \beta_2 = ... = \beta_d = B_k$.
Let E_1 be the set of all edges which are incident with the center vertex, $|E_1| = d$. Let E_2 be the set of all edges which are incident with the root of B_k which has degree $k+1$ and

the vertex of degree two, $|E_2| = k|B_k|$. Let E_3 be the set of all edges which are incident with the vertex of degree two and vertex of degree one, $|E_3| = k|B_k|$.

$$\begin{aligned}
VD(T,x) &= \sum_{uv\in E(T)} d(u)x^{d(v)} \\
&= \sum_{uv\in E_1}(dx^{k+1}+(k+1)x^d) + \sum_{uv\in E_2}((k+1)x^2+2x^{k+1}) + \sum_{uv\in E_3}(x^2+2x) \\
&= d(dx^{k+1}+(k+1)x^d) + k|B_k|((k+1)x^2+2x^{k+1}) + k|B_k|(x^2+2x) \\
&= d(k+1)x^d + (d^2+2k|B_k|)x^{k+1} + k(k+2)|B_k|x^2 + 2k|B_k|x.
\end{aligned}$$

Case (2) If $\beta_1 \cong B_s$, $\beta_2 \cong B_r$, ..., $\beta_d \cong B_k$, and $|B_s| = |B_r| = ... = |B_k| = 1$

Let E_1 be the set of all edges which are incident with the center vertex, $|E_1| = d$. Let E_2 be the set of all edges which are incident with the root of B_s which has degree $s+1$ and the vertex of degree two, $|E_2| = s$. Let E_3 be the set of all edges which are incident with the root of B_r which has degree $r+1$ and the vertex of degree two, $|E_3| = r$.

⋮

E_k be the set of all edges which are incident with the root of B_k which has degree $k+1$ and the vertex of degree two, $|E_k| = k$. Let E_p be the set of all edges which are incident with the vertex of degree two and vertex of degree one, $|E_p| = s+r+...+k$.

$$\begin{aligned}
VD(T,x) &= \sum_{uv\in E(T)} d(u)x^{d(v)} \\
&= \sum_{uv\in E_1-(d-1)}(dx^{s+1}+(s+1)x^d) + \sum_{uv\in E_1-(d-1)}(dx^{r+1}+(r+1)x^d) + ... \\
&+ \sum_{uv\in E_1-(d-1)}(dx^{k+1}+(k+1)x^d) + \sum_{uv\in E_2}((s+1)x^2+2x^{s+1}) + \sum_{uv\in E_3}((r+1)x^2+2x^{r+1}) \\
&+ ... + \sum_{uv\in E_k}((k+1)x^2+2x^{k+1}) + \sum_{uv\in E_p}(x^2+2x) \\
&= (dx^{s+1}+(s+1)x^d) + (dx^{r+1}+(r+1)x^d) + ... + (dx^{k+1}+(k+1)x^d) \\
&+ s((s+1)x^2+2x^{s+1}) + r((r+1)x^2+2x^{r+1}) + ... + (s+r+...+k)(x^2+2x).
\end{aligned}$$

Case (3) If $\beta_1 \cong B_s$, $\beta_2 \cong B_r$,...,, $\beta_{d-1} \cong B_z$, $\beta_d \cong B_k$, and $|B_s| = i$, $|B_r| = j$,..., $|B_z| = g$, $|B_k| = h$.

Let $E_1 = d = i+j+...+h$ be the set of all edges which are adjacent with the center vertex. $E_2 = s|B_s|$ be the set of all edges which are adjacent with the root of B_s which has degree $s+1$ and the vertex of degree two. $E_3 = r|B_r|$ be the set of all edges which are adjacent with the root of B_r which has degree $r+1$ and the vertex of degree two.

⋮

$E_k = k|B_k|$ be the set of all edges which are adjacent with the root of B_k which has degree $k+1$ and the vertex of degree two. $E_p = s|B_s| + r|B_r| + ... + k|B_k|$ be the set of all edges which are adjacent with the vertex of degree two and vertex of degree one.

$$
\begin{aligned}
VD(T,x) &= \sum_{uv\in E(T)} d(u)x^{d(v)} \\
&= \sum_{uv\in E_1-(j+l+...+h)} ((dx^{s+1}+(s+1)x^d)) + \sum_{uv\in E_1-(i+l+...+h)} ((dx^{r+1}+(r+1)x^d)) \\
&+ ... + \sum_{uv\in E_1-(i+j+l+...+g)} ((dx^{k+1}+(k+1)x^d)) + \sum_{uv\in E_2} ((s+1)x^2+2x^{s+1}) \\
&+ \sum_{uv\in E_3} ((r+1)x^2+2x^{r+1}) + ... + \sum_{uv\in E_k} ((k+1)x^2+2x^{k+1}) + \sum_{uv\in E_p} (x^2+2x) \\
&= |d-(j+l+...+h)|(dx^{s+1}+(s+1)x^d) + |d-(i+l+...+h)|(dx^{r+1}+(r+1)x^d) + ... \\
&+ |d-(i+j+...+g)|(dx^{k+1}+(k+1)x^d) + s|B_s|((s+1)x^2+2x^{s+1}) \\
&+ r|B_r|((r+1)x^2+2x^{r+1}) + ... + k|B_k|((k+1)x^2+2x^{k+1}) \\
&+ [s|B_s|+r|B_r|+...+k|B_k|](x^2+2x) \\
&= i(dx^{s+1}+(s+1)x^d) + j(dx^{r+1}+(r+1)x^d) + ... + h(dx^{k+1}+(k+1)x^d) \\
&+ s|B_s|((s+1)x^2+2x^{s+1}) + r|B_r|((r+1)x^2+2x^{r+1}) + ... + k|B_k|((k+1)x^2+2x^{k+1}) \\
&+ [s|B_s|+r|B_r|+...+k|B_k|](x^2+2x).
\end{aligned}
$$

□

Lemma 3.1. *Let $N(v)$ be the set of all neighborhood of the vertex v in $G=(V,E)$. The vertex degree polynomial of G is given by $VD(G,x)=\sum_{v\in V(G)} d_N(v)x^{d(v)}$, where $d_N(v)=\sum_{u\in N(v)} d(u)$*

The Sierpiński triangle S_j is a fixed set with the overall shape of an equilateral triangle, subdivided recursively into smaller equilateral triangles. The graph S_j has $\frac{3}{2}(3^{j-1}+1)$ vertices and 3^j edges.

Proposition 3.2. *The vertex degree polynomial of the Sierpinski sieve graph S_j is given by $VD(S_j,x)=24x^2+((3^j)8-36)x^4$. Further,*

$$Z_{VD}(VD(S_j,x))=\{0,\sqrt{\frac{-24}{(3^j)8-36}}\}.$$

Proof. The proof is produced directly from Lemma 3.1. □

Definition 3.4. *A polynomial $P(x)$ is called graphical vertex degree polynomial if there exists at least one simple graph G such that $VD(G,x)=P(x)$.*

Definition 3.5. *Two graphs G_1 and G_2 are called equal vertex degree polynomial if and only if $VD(G_1,x)=VD(G_2,x)$.*

Observation 3.2.

(1) *There is no vertex degree polynomial in which all the coefficients are* 1.
(2) *The summation of all the coefficients of the vertex degree polynomial is even.*

Proof. (1) There is no graph with all vertices are of degree one except P_2 and in P_2 the vertex degree polynomial is $2x$. So, there is no vertex degree polynomial in which all the coefficients are 1.

(2) The summation of the coefficients of vertex degree polynomial is two times the summation of the degree of the vertices which is $4m$.

□

Observation 3.3.
If G_1 and G_2 are any two graphs such that $G_1 \cong G_2$, then

$$VD(G_1, x) = VD(G_2, x).$$

The converse is not true because sometimes $G_1, G_2, ..., G_s$ are not isomorphic, but they have the same vertex degree polynomial, i.e if $VD(G_1, x) = VD(G_2, x)$, then it does not mean that $G_1 \cong G_2$.

This is explained in the following example:

Example 3.2. *Let G_1 and G_2 be two non isomorphic graphs as in Fig 6, so clearly G_1 and G_2 are non isomorphic graphs, but $VD(G_1, x) = VD(G_2, x) = 6x^3 + 18x^2 + 2x$.*

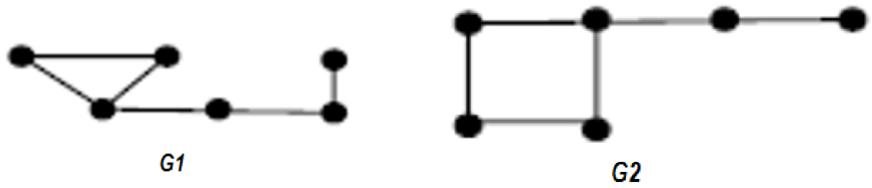

FIGURE 6. Plotting of (a) Graph G_1 and (b) Graph G_2

Theorem 3.7. *Let G be a connected graph with n vertices. Then*

(1) *There is no vertex degree polynomial of the form x^n.*
(2) *Zero is a vertex degree root of $VD(G, x)$.*
(3) *$VD(G, x)$ has no constant term.*
(4) *$VD(G, x)$ is strictly increasing function on $[0, \infty)$.*

Proof. (1) As the maximum degree for any graph of n vertices is n-1.
(2) As each term in the polynomial contains at least x of the power one.
(3) For any connected graph G, $\delta(G) \geq 1$.
(4) The derivative is always greater than zero .

□

4. Applications

In this section, we apply Theorem 3.1 to calculate the second Zagreb index for Dyck-56 network and also for the chemical compound triangular benzenoid $G[r]$.

Example 4.1. *Let G be the molecule graph of $Dyck - 56_{s\times s}(A)$ as in Fig 7. Then $VD(G, x) = (108s - 44)sx^3 + 40sx^2$, and $Z_{VD}(G, x) = \{0, \frac{-40}{108s-44}\}$.*
The edge sets of $Dyck - 56_{s\times s}(A)$ can be divided into three types as follows:

$$E_1(G) = \{uv \in E(G) : d(u) = 2 \ \text{and} \ d(v) = 2\},$$
$$E_2(G) = \{uv \in E(G) : d(u) = 2 \ \text{and} \ d(v) = 3\},$$
$$E_3(G) = \{uv \in E(G) : d(u) = 3 \ \text{and} \ d(v) = 3\}.$$

Note that $|E_1(G)| = 4s$, $|E_2(G)| = 8s$ *and* $|E_3(G)| = 2s(9s-5)$.
By using Theorem 3.1, we get

$$M_1(G) = (108s - 4)s,$$

$$M_2(G) = 3s(54s - 22) + 40s,$$

$$D_x^2(VD(G,x))|_{x=1} = 648s^2 - 184s.$$

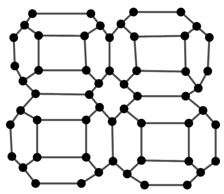

FIGURE 7. $Dyck - 56_{2\times 2}(A)$

Example 4.2. *Suppose G be the molecule graph of* $Dyck - 56_{s\times s}(B)$ *as in Fig 8, then* $VD(G,x) = 36s(s-1)x^4 + (120s^2 - 32s + 16)x^3 + 24(s+1)x^2$, *and*

$$Z_{VD}(G,x) = \{0, \frac{-(15s^2 - 4s + 2) \pm \sqrt{225s^4 - 174s^3 + 76s^2 + 38s + 4}}{9s(s-1)}\}.$$

Also, the edge sets of $Dyck - 56_{s\times s}(B)$ *can be divided into three types as follows:*

$$E_1(G) = \{uv \in E(G) : d(u) = 2 \ \ and \ \ d(v) = 3\},$$

$$E_2(G) = \{uv \in E(G) : d(u) = 3 \ \ and \ \ d(v) = 3\},$$

$$E_3(G) = \{uv \in E(G) : d(u) = 3 \ \ and \ \ d(v) = 4\}.$$

Note that $|E_1(G)| = 8(s+1)$, $|E_2(G)| = 12s^2$ *and* $|E_3(G)| = 12s(s-1)$.
Using Theorem 3.1, we get

$$M_1(G) = (156s - 44)s + 40,$$

$$M_2(G) = 72s(s-1) + 12(15s^2 - 4s + 2) + 24(s+1),$$

$$D_x^2(VD(G,x))|_{x=1} = 1152s^2 - 576s + 144.$$

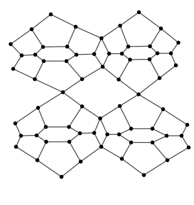

FIGURE 8. $Dyck - 56_{s\times s}(B)$

Example 4.3. *Let $G[r]$ be the molecule structure of triangular benzenoid as Fig 9. Then $VD(G[r],x) = (r-1)(12+9r)x^3 + 6(3r+1)x^2$, and $Z_{VD}(G[r],x) = \{0, \frac{-6(3r+1)}{(r-1)(12+9r)}\}$. The edge sets of $G[r]$ can be divided into three types as follows:*

$$E_1(G[r]) = \{uv \in E(G[r]) : d(u) = 2 \ \ and \ \ d(v) = 2\},$$
$$E_2(G[r]) = \{uv \in E(G[r]) : d(u) = 2 \ \ and \ \ d(v) = 3\},$$
$$E_3(G[r]) = \{uv \in E(G[r]) : d(u) = 3 \ \ and \ \ d(v) = 3\}.$$

Note that $|E_1(G[r])| = 6$, $|E_2(G[r])| = 6(r-1)$ and $|E_3(G[r])| = \frac{3r}{2}(r-1)$.
Using Theorem 3.1, we get

$$M_1(G[r]) = 9r^2 + 21r - 6,$$
$$M_2(G[r]) = \frac{3(r-1)(12+9r) + 12(3r+1)}{2},$$
$$D_x^2(VD(G[r],x))|_{x=1} = 54r^2 + 54r - 60.$$

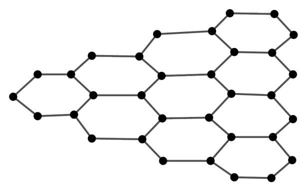

FIGURE 9. $G[4]$

5. Conclusions

In this paper, new graph polynomial, called vertex degree polynomial is introduced and its chemical importance is presented by studying the relations between the coefficients of the polynomial and its derivatives with the topological indices and studying the correlation of the summation of the coefficients of second derivative of the vertex degree polynomial for the isomers of octanes with some chemical properties. We have calculated the vertex degree polynomial along with its roots for some important families of graphs. Finally, using the vertex degree polynomial, similarly, the first and second Zagreb indices for Dyck-56 network and also for the chemical compound triangular benzenoid are calculated. It would be of great interest if we can identify a graph on the basis of a given polynomial. This will further give rise to many more interesting results.

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Hanan Ahmed graduated in Mathematics and got her MSc degree in Mathematics in 2018 from Savitribai Phule Pune University, Pune, India. Presently, she is working as a research scholar of Mathematics in the Department of Mathematics at Yuvarajs College, University of Mysore, Mysore, India. Her research interests are topological indices, polynomial of graphs, and chemical graph theory.

Anwar Alwardi is an assistant professor at the University of Aden, Yemen. He got his MSc degree in Mathematics in September 2009, from King Abdulaziz University, Saudi Arabia, and his Ph.D. degree in Mathematics in October 2014 from the University of Mysore, Mysore, India. His research interests are Algebra, Graph Theory and Design Theory and their applications in all sciences.

Ruby Salestina M. obtained her MSc degree in Mathematics in 1999 from the University of Mysore, India. She was awarded her Ph.D degree in Mathematics from the same University in the year 2003. Her recent areas of research include Theory of Numbers, Graph Theory and Geometric Function Theory. Presently, she is working as an associate professor in the Department of Mathematics, Yuvaraja's College, University of Mysore, India.