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ON THE VERTEX-EDGE WIENER INDICES OF THORN GRAPHS

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Abstract. The vertex-edge Wiener index is a graph invariant defined as the sum of distances between vertices and edges of a graph. In this paper, we study the relation between the first and second vertex-edge Wiener indices of thorn graph and its parent graph and examine several special cases of the results. Results are applied to compute the first and second vertex-edge Wiener indices of thorn stars, Kragujevac trees, and dendrimers.

1. Introduction

All graphs considered in this paper are finite, simple and connected. Let G be an n-vertex graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and let $\mathrm{P} = (p_1, p_2, \dots, p_n)$ be an n-tuple of nonnegative integers. The *thorn graph* G_{P} is the graph obtained by attaching p_i pendent vertices (terminal vertices or vertices of degree one) to the vertex v_i of G, for $i = 1, 2, \dots, n$. The p_i pendent vertices attached to the vertex v_i are called thorns of v_i, $i = 1, 2, \dots, n$. We denote the set of p_i thorns of v_i by V_i and the set of p_i edges connecting the vertex v_i and its thorns by E_i, $i = 1, 2, \dots, n$. Clearly, $V(G_{\mathrm{P}}) = V(G) \cup V_1 \cup V_2 \cup \dots \cup V_n$ and $E(G_{\mathrm{P}}) = E(G) \cup E_1 \cup E_2 \cup \dots \cup E_n$, and for $1 \le i \ne j \le n$, $V_i \cap V_j = E_i \cap E_j = \phi$. The concept of thorn graphs was introduced in 1998 by Gutman [9] and eventually found a variety of chemical applications; see, e.g., [3]. The motivation for the study of thorn graphs came from a particular case, namely $G_{\mathrm{P}} = G_{(\gamma-\gamma_1, \gamma-\gamma_2, \dots, \gamma-\gamma_n)}$, where γ_i is the degree of the i-th vertex of G and γ is a constant ($\gamma \ge \gamma_i$ for all $i = 1, 2, \dots, n$). Then the vertices of G_{P} are either of degree γ or of degree one. If in addition $\gamma = 4$, then the thorn graph G_{P} is just what Cayley [6] calls a *plerogram* (a graph in which every atom is represented by a vertex and adjacent atoms are connected by a chemical bond) and Polya [14] a *C-H graph.* The parent graph G would then be referred to as a *kenogram* [6] (a graph obtained from a plerogram by suppressing hydrogen atoms) or a *C-graph* [14] .

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A *topological index* is a numeric quantity that is mathematically derived in a direct and unambiguous manner from the structural graph of a molecule. It is used in theoretical chemistry for the design of chemical compounds with given physico-chemical properties or given pharmacologic and biological activities [16]. It is well known that the study of topological indices of kenograms is much more conventional than plerograms, because of their simplicity and the fact that many topological indices give highly correlated results on plerograms and kenograms [11]. The study of thorn graphs unifies these two approaches by giving mathematical formulae that connect the values of topological indices of kenograms and plerograms.

In this paper, we study the relation between the first and second vertex-edge Wiener indices of a graph and its thorn graph and examine several special cases of the results. Results are applied to compute the first and second vertex-edge Wiener indices of thorn stars, Kragujevac trees, and a class of dendrimers.

2. Definitions and preliminaries

In this paper, we consider connected finite graphs without any loops or multiple edges. The best known and widely used topological index is the *Wiener index* introduced by Wiener [17] in 1947, who used it for modeling the shape of organic molecules and for calculating several of their physico-chemical properties. The Wiener index of a graph G is defined as the sum of distances between all pairs of vertices of G,

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

where $d(u,v|G)$ denotes the distance between the vertices u and v in G.

The *degree distance* was introduced in 1994 by Dobrynin and Kochetova [7] and at the same time by Gutman [8] as a weighted version of the Wiener index. The degree distance of a graph G is defined as

$$DD(G) = \sum_{\{u,v\}\subseteq V(G)} [d_G(u) + d_G(v)]d(u,v|G),$$

where $d_G(u)$ denotes the degree of the vertex u in G.

The *Gutman index* (also known as *Schultz index of the second kind*) was introduced in 1994 by Gutman [8] as a kind of vertex-valency-weighted sum of the distances between all pairs of vertices in a graph. The Gutman index of a graph G is defined as

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u)d_G(v)d(u,v|G).$$

The concept of *terminal Wiener index* was put forward by Gutman et al. [12] in 2009. Somewhat later, but independently, Székely *et al.* [15] arrived at the same idea. The terminal Wiener index $TW(G)$ of a graph G is defined as the sum of distances between all pairs of its pendent vertices,

$$TW(G) = \sum_{\{u,v\}\subseteq V'(G)} d(u,v|G),$$

where $V'(G)$ is the set of all pendent vertices of G.

For $u \in V(G)$, we define the quantity $TW_G(u)$ as the sum of distances between u and all pendent vertices of G,

$$TW_G(u) = \sum_{v \in V'(G)} d(u, v|G).$$

It is easy to see that, $TW(G) = \frac{1}{2} \sum_{u \in V'(G)} TW_G(u)$.

In analogy with definition of the Wiener index, the vertex-edge Wiener indices [2, 5, 13] were defined based on distances between vertices and edges of a graph. The distances $D_1(u, e|G)$ and $D_2(u, e|G)$ between the vertex u and edge $e = ab$ of a graph G are defined as

$$D_1(u, e|G) = \min\{d(u, a|G), d(u, b|G)\}, \quad D_2(u, e|G) = \max\{d(u, a|G), d(u, b|G)\}.$$

The first and second vertex-edge Wiener indices of G are denoted by $W_{ve_1}(G)$ and $W_{ve_2}(G)$, respectively and defined as

$$W_{ve_i}(G) = \sum_{u \in V(G)} \sum_{e \in E(G)} D_i(u, e|G), \quad i \in \{1, 2\}.$$

For $u \in V(G)$, we define

$$D_i(u|G) = \sum_{e \in E(G)} D_i(u, e|G), \quad i \in \{1, 2\}.$$

Then, the first and second vertex-edge Wiener indices of G can also be expressed by

$$W_{ve_i}(G) = \sum_{u \in V(G)} D_i(u|G), \quad i \in \{1, 2\}.$$

The relation between the first and second vertex-edge Wiener indices of bipartite graphs was given in [1].

Theorem 2.1 ([1]). *A simple connected graph G of order n and size m is bipartite if and only if $W_{ve_2}(G) = W_{ve_1}(G) + nm$.*

We refer the reader to [1, 4] for more information on vertex-edge Wiener indices.

3. Results and disscusion

In this section, we establish the relation between the first and second vertex-edge Wiener indices of a graph G and its thorn graph G_{P}, and examine several special cases of the result.

Theorem 3.1. *Let G be a graph of order n and size m with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, and let G_{P} be the thorn graph of G with nonnegative parameters $p_1, p_2, \ldots, p_n$. Then*

$$W_{ve_r}(G_P) = W_{ve_r}(G) + (m + n(r-1) - 1) \sum_{i=1}^{n} p_i + r(\sum_{i=1}^{n} p_i)^2 + \sum_{i=1}^{n} p_i D_r(v_i|G)$$

$$+\sum_{1\le i<j\le n}(p_i+p_j)d(v_i,v_j|G)+2\sum_{1\le i<j\le n}p_ip_jd(v_i,v_j|G), \tag{1}$$

where $r\in\{1,2\}$.

Proof. By definition of the vertex-edge Wiener indices, we have

$$W_{ve_r}(G_{\rm P})=\sum_{u\in V(G_{\rm P})}\sum_{e\in E(G_{\rm P})}D_r(u,e|G_P),\quad r\in\{1,2\}.$$

By definition of the graph $G_{\rm P}$, the above sum can be partitioned into four sums as follows.

The first sum S_1 is taken over all vertices $u\in V(G)$ and edges $e\in E(G)$. In this case, $D_r(u,e|G_P)=D_r(u,e|G)$, $r\in\{1,2\}$. So, for $r\in\{1,2\}$ we have

$$S_1=\sum_{u\in V(G)}\sum_{e\in E(G)}D_r(u,e|G_P)=\sum_{u\in V(G)}\sum_{e\in E(G)}D_r(u,e|G)=W_{ve_r}(G).$$

The second sum S_2 is taken over all vertices $u=v_i\in V(G)$, $1\le i\le n$ and edges $e\in E_j$, $1\le j\le n$. In this case, $D_r(u,e|G_P)=d(v_i,v_j|G)+r-1$, $r\in\{1,2\}$. So, for $r\in\{1,2\}$ we have

$$S_2=\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{e\in E_j}[d(v_i,v_j|G)+r-1]=\sum_{i=1}^{n}\sum_{j=1}^{n}p_j[d(v_i,v_j|G)+r-1]$$

$$=\sum_{1\le i<j\le n}(p_i+p_j)d(v_i,v_j|G)+n(r-1)\sum_{i=1}^{n}p_i.$$

The third sum S_3 is taken over all vertices $u\in V_i$, $1\le i\le n$ and edges $e\in E(G)$. In this case, $D_r(u,e|G_P)=1+D_r(v_i,e|G)$, $r\in\{1,2\}$. So, for $r\in\{1,2\}$ we have

$$S_3=\sum_{i=1}^{n}\sum_{u\in V_i}\sum_{e\in E(G)}[1+D_r(v_i,e|G)]=m\sum_{i=1}^{n}p_i+\sum_{i=1}^{n}p_iD_r(v_i|G).$$

The fourth sum S_4 is taken over all vertices $u\in V_i$, $1\le i\le n$ and edges $e\in E_j$, $1\le j\le n$. If $e=uv_i$, then $D_r(u,e|G_P)=r-1$; otherwise, $D_r(u,e|G_P)=r+d(v_i,v_j|G)$, $r\in\{1,2\}$. So, for $r\in\{1,2\}$ we have

$$S_4=\sum_{i=1}^{n}\sum_{u\in V_i}\Big[(r-1)+\sum_{e\in E_i,e\neq uv_i}r+\sum_{i\neq j=1}^{n}\sum_{e\in E_j}[r+d(v_i,v_j|G)]\Big]$$

$$=(r-1)\sum_{i=1}^{n}p_i+r\sum_{i=1}^{n}p_i(p_i-1)+\sum_{i=1}^{n}\sum_{i\neq j=1}^{n}\sum_{u\in V_i}\sum_{e\in E_j}[r+d(v_i,v_j|G)]$$

$$=(r-1)\sum_{i=1}^{n}p_i+r\sum_{i=1}^{n}p_i(p_i-1)+r\sum_{i=1}^{n}\sum_{i\neq j=1}^{n}p_ip_j+\sum_{i=1}^{n}\sum_{i\neq j=1}^{n}p_ip_jd(v_i,v_j|G)$$

$$=r\sum_{i=1}^{n}p_i^2-\sum_{i=1}^{n}p_i+r(\sum_{i=1}^{n}p_i)^2-r\sum_{i=1}^{n}p_i^2+\sum_{i=1}^{n}\sum_{i\neq j=1}^{n}p_ip_jd(v_i,v_j|G)$$

$$= r(\sum_{i=1}^{n} p_i)^2 - \sum_{i=1}^{n} p_i + 2 \sum_{1\leq i<j\leq n} p_i p_j d(v_i, v_j|G).$$

(1) is obtained by adding S_1, S_2, S_3, S_4, and simplifying the resulting expression. □

For any connected graph G, we define the quantity $\alpha(G)$ as the sum of distances between all non pendent vertices of G and its pendent vertices,

$$\alpha(G) = \sum_{u\in V(G)-V'(G)} TW_G(u).$$

In the following theorem, we find a formula for $\alpha(G_P)$.

THEOREM 3.2. *Let G be an n-vertex graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$, and let G_{P} be the thorn graph of G with parameters $p_1, p_2, \ldots, p_n$ such that for every pendent vertex v_i of G, $p_i > 0$. Then*

$$\alpha(G_P) = \sum_{1\leq i<j\leq n} (p_i + p_j) d(v_i, v_j|G) + n \sum_{i=1}^{n} p_i. \tag{2}$$

Proof. Since for every pendent vertex v_i of G, $p_i > 0$, so $V'(G_P) = V_1 \cup V_2 \cup \ldots \cup V_n$ and $V(G_P) - V'(G_P) = V(G)$. Then

$$\alpha(G_P) = \sum_{u\in V(G)} TW_{G_P}(u) = \sum_{u\in V(G)} \sum_{v\in V_1\cup\ldots\cup V_n} d(u, v|G_P)$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{v\in V_j} (d(v_i, v_j|G) + 1) = \sum_{i=1}^{n}\sum_{j=1}^{n} p_j (d(v_i, v_j|G) + 1)$$

$$= \sum_{1\leq i<j\leq n} (p_i + p_j) d(v_i, v_j|G) + n \sum_{i=1}^{n} p_i,$$

which completes the proof. □

As a direct consequence of Theorem 3.2, we get the following corollary which will be used in the next section.

COROLLARY 3.3. *Let G be an n-vertex graph with k pendent vertices, and let G_{P} be the thorn graph of G obtained by attaching $p > 0$ pendent vertices to each pendent vertex of G. Then*

$$\alpha(G_P) = 2pTW(G) + p\alpha(G) + knp. \tag{3}$$

Proof. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$, and without loss of generality let $V'(G) = \{v_1, v_2, \ldots, v_k\}$. By setting $p_1 = p_2 = \ldots = p_k = p$ and $p_{k+1} = p_{k+2} = \ldots = p_n = 0$ in (2), we obtain

$$\alpha(G_P) = \sum_{1\leq i<j\leq k} (p + p) d(v_i, v_j|G) + \sum_{k+1\leq i<j\leq n} (0 + 0) d(v_i, v_j|G)$$

$$+ \sum_{i=1}^{k}\sum_{j=k+1}^{n} (p + 0) d(v_i, v_j|G) + n\big(\sum_{i=1}^{k} p + \sum_{i=k+1}^{n} 0\big).$$

We get (3) using the facts that

$$\sum_{1\le i<j\le k} d(v_i,v_j|G)=TW(G) \quad \text{and} \quad \sum_{i=1}^{k}\sum_{j=k+1}^{n} d(v_i,v_j|G)=\alpha(G).$$

□

Now, we express some special cases of Theorem 3.1.

COROLLARY 3.4. *Let G be a graph of order n and size m, and let G_{P} be the thorn graph of G with parameters $p_1=p_2=\ldots=p_n=p$, where p is a nonnegative integer. Then*

$$W_{ve_r}(G_{\mathrm{P}})=(p+1)W_{ve_r}(G)+2p(p+1)W(G)+np\big(n(rp+r-1)+m-1\big),$$

where $r\in\{1,2\}$.

COROLLARY 3.5. *Let G be a graph of order n and size m with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$, and let $v_1,v_2,\ldots,v_k$ be its pendent vertices. Suppose G_{P} is the thorn graph of G with parameters $p_1,p_2,\ldots,p_n$, such that $p_i=\begin{cases} p & if\ 1\le i\le k,\\ 0 & if\ k+1\le i\le n,\end{cases}$ where p is a nonnegative integer. Then*

$$\begin{aligned}W_{ve_r}(G_{\mathrm{P}})=W_{ve_r}(G)&+2p(p+1)TW(G)+kp\big(n(r-1)+m-1+rkp\big)\\ &+p\alpha(G)+p\sum_{i=1}^{k}D_r(v_i|G),\end{aligned} \tag{4}$$

where $r\in\{1,2\}$.

COROLLARY 3.6. *Let G be a graph of order n and size m with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$, and let G_{P} be the thorn graph of G with parameters $p_1,p_2,\ldots,p_n$, where $p_i=d_G(v_i)$, $i=1,2,\ldots,n$. Then*

$$\begin{aligned}W_{ve_r}(G_{\mathrm{P}})=W_{ve_r}(G)&+DD(G)+2Gut(G)+2m\big(n(r-1)+m(2r+1)-1\big)\\ &+\sum_{i=1}^{n}d_G(v_i)D_r(v_i\,|G),\quad r\in\{1,2\}.\end{aligned}$$

Proof. It is easy to see that, $\sum_{i=1}^{n}p_i=2m$, $\sum_{1\le i<j\le n}(p_j+p_i)d(v_i,v_j|G)=DD(G)$, and $\sum_{1\le i<j\le n}p_ip_jd(v_i,v_j\,|G)=Gut(G)$. Now using (1), we can get the desired result. □

COROLLARY 3.7. *Let G be a graph of order n and size m with vertex set $V(G)=\{v_1,v_2,\ldots,v_n\}$, and let γ be an integer with the property $\gamma\ge d_G(v_i)$, for $i=1,2,\ldots,n$. Let G_{P} be the thorn graph of G with parameters $p_1,p_2,\ldots,p_n$, where $p_i=\gamma-d_G(v_i)$, $i=1,2,\ldots,n$. Then*

$$\begin{aligned}W_{ve_r}(G_{\mathrm{P}})=(\gamma+1)W_{ve_r}(G)&+2\gamma(\gamma+1)W(G)-(2\gamma+1)DD(G)+2Gut(G)\\ &+(n\gamma-2m)\big(r(n\gamma-2m)+m+n(r-1)-1\big)-\sum_{i=1}^{n}d_G(v_i)D_r(v_i|G),\end{aligned}$$

where $r\in\{1,2\}$.

Proof. It is easy to see that,

$$\sum_{i=1}^{n} p_i = n\gamma - 2m,$$

$$\sum_{i=1}^{n} p_i D_r(v_i|G) = \gamma W_{ve_r}(G) - \sum_{i=1}^{n} d_G(v_i) D_r(v_i|G),$$

$$\sum_{1\le i<j\le n} (p_j + p_i) d(v_i, v_j|G) = 2\gamma W(G) - DD(G),$$

$$\sum_{1\le i<j\le n} p_i p_j d(v_i, v_j|G) = \gamma^2 W(G) - \gamma DD(G) + Gut(G).$$

Now using (1), we can get the desired result. □

4. Applications

In this section, we apply the results of the previous section, to compute the vertex-edge Wiener indices of thorn stars, Kragujevac trees, and a class of dendrimers.

4.1 Thorn stars

Consider the star graph S_{d+1} and choose a labelling for its vertices such that its terminal vertices have numbers $1, 2, \ldots, d$ and its central vertex has number $d+1$. Let $S_{d+1}(p_1, p_2, \ldots, p_d)$ denote the *thorn star* obtained by attaching p_i terminal vertices to vertex i of S_{d+1} for $1, 2, \ldots, d$ (see Figure 1).

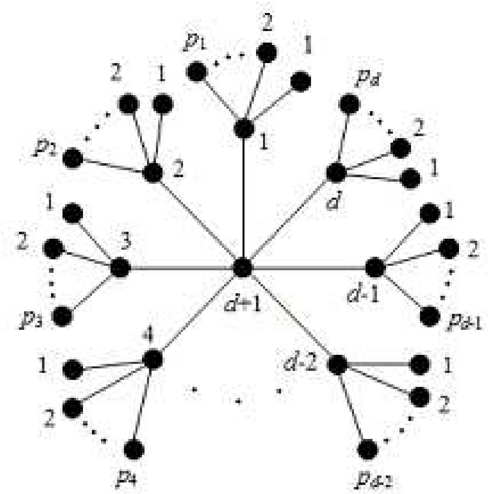

Figure 1: The thorn star $S_{d+1}(p_1, p_2, \ldots, p_d)$.

THEOREM 4.1. *Let $d \geq 2$ and let $p_1, p_2 \ldots, p_d$ be nonnegative integers. Then*

$$W_{ve_1}\big(S_{d+1}(p_1,p_2,\ldots,p_d)\big) = d(d-1) + 3(\sum_{i=1}^{d} p_i)^2 - 2\sum_{i=1}^{d} p_i^2 + (4d-3)\sum_{i=1}^{d} p_i, \quad (5)$$

$$W_{ve_2}\big(S_{d+1}(p_1,p_2,\ldots,p_d)\big) = 2d^2 + 4(\sum_{i=1}^{d} p_i)^2 - 2\sum_{i=1}^{d} p_i^2 + (6d-2)\sum_{i=1}^{d} p_i. \quad (6)$$

Proof. By setting $G = S_{d+1}$, $G_P = S_{d+1}(p_1,p_2,\ldots,p_d)$, $p_{d+1} = 0$, $n = d+1$, and $m = d$ in (1), we obtain

$$W_{ve_1}\big(S_{d+1}(p_1,p_2,\ldots,p_d)\big) = W_{ve_1}(S_{d+1}) + (d-1)\sum_{i=1}^{d} p_i + (\sum_{i=1}^{d} p_i)^2 + \sum_{i=1}^{d} p_i D_1(v_i|S_{d+1})$$
$$+ 2\sum_{1\leq i<j\leq d}(p_i+p_j) + \sum_{1\leq i\leq d, j=d+1}(p_i+0) + 4\sum_{1\leq i<j\leq d} p_i p_j + 2\sum_{1\leq i\leq d, j=d+1}(p_i \times 0), \quad (7)$$

where v_i, $1 \leq i \leq d$, is the vertex of S_{d+1} whose number is i. It is easy to see that, $W_{ve_1}(S_{d+1}) = d(d-1)$, $D_1(v_i|S_{d+1}) = d-1$, $1 \leq i \leq d$, $2\sum_{1\leq i<j\leq d}(p_i+p_j) = (2d-2)\sum_{i=1}^{d} p_i$, and $2\sum_{1\leq i<j\leq d} p_i p_j = (\sum_{i=1}^{d} p_i)^2 - \sum_{i=1}^{d} p_i^2$. By substituting these relations in (7) and simplifying the resulting expression, we can get (5). To prove (6), note that the thorn star $S_{d+1}(p_1,p_2,\ldots,p_d)$ is a bipartite graph with $\sum_{i=1}^{d} p_i + d + 1$ vertices and $\sum_{i=1}^{d} p_i + d$ edges. So, by Theorem 2.1,

$$W_{ve_2}\big(S_{d+1}(p_1,p_2,\ldots,p_d)\big) = W_{ve_1}\big(S_{d+1}(p_1,p_2,\ldots,p_d)\big) + (\sum_{i=1}^{d} p_i + d + 1)(\sum_{i=1}^{d} p_i + d).$$

Now using (5) and simplifying the resulting expression, we can get (6). □

4.2 Kragujevac trees

Let P_3 be the 3-vertex path rooted at one of its terminal vertices. For $k \geq 2$, 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. Examples illustrating the structure of the rooted tree B_k are depicted in Figure 2.

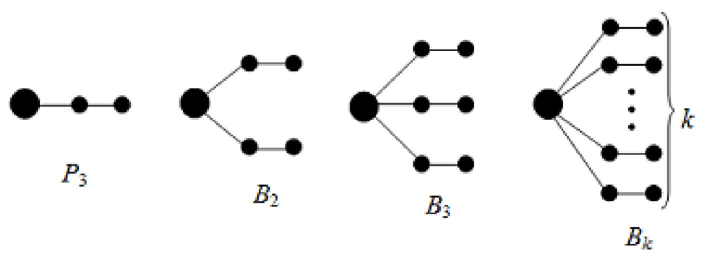

Figure 2: The rooted trees B_2, B_3, and B_k. Their roots are indicated by large dots.

According to [10], a *Kragujevac tree* T is a tree possessing a vertex of degree $d \geq 2$, adjacent to the roots of $B_{p_1}, B_{p_2}, \ldots, B_{p_d}$, where $p_1, p_2, \ldots, p_d \geq 2$. This vertex is said to be the central vertex of T, whereas d is the degree of T. The subgraphs $B_{p_1}, B_{p_2}, \ldots, B_{p_d}$ are the branches of T. Note that some (or all) branches of T may be mutually isomorphic. We denote the Kragujevac tree of degree d with branches $B_{p_1}, B_{p_2}, \ldots, B_{p_d}$ by $Kg(p_1, p_2, \ldots, p_d)$. A typical Kragujevac tree is depicted in Figure 3.

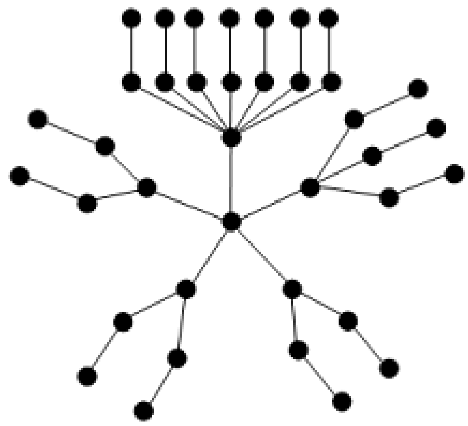

Figure 3: The Kragujevac tree $Kg(7, 3, 2, 2, 2)$.

Theorem 4.2. *The first and second vertex-edge Wiener indices of the Kragujevac tree $Kg(p_1, p_2, \ldots, p_d)$ are given by*

$$W_{ve_1}\big(Kg(p_1, p_2, \ldots, p_d)\big) = d(d-1) + 16(\sum_{i=1}^{d} p_i)^2 - 8\sum_{i=1}^{d} p_i^2 + 10(d-1)\sum_{i=1}^{d} p_i, \quad (8)$$

$$W_{ve_2}\big(Kg(p_1, p_2, \ldots, p_d)\big) = 2d^2 + 20(\sum_{i=1}^{d} p_i)^2 - 8\sum_{i=1}^{d} p_i^2 + (14d-8)\sum_{i=1}^{d} p_i. \quad (9)$$

Proof. The Kragujevac tree $Kg(p_1, p_2, \ldots, p_d)$ can be considered as the thorn graph obtained from the thorn star $S_{d+1}(p_1, p_2, \ldots, p_d)$ by attaching a pendent vertex to each of its pendent vertices. Now, by setting $G = S_{d+1}(p_1, p_2, \ldots, p_d)$, $G_P = Kg(p_1, \ldots, p_d)$, $p = 1$, $k = \sum_{i=1}^{d} p_i$, and $m = \sum_{i=1}^{d} p_i + d$ in (4), we obtain

$$W_{ve_1}\big(Kg(p_1, \ldots, p_d)\big) = W_{ve_1}\big(S_{d+1}(p_1, \ldots, p_d)\big) + 4TW\big(S_{d+1}(p_1, \ldots, p_d)\big) \quad (10)$$
$$+ \sum_{i=1}^{d} p_i\big(2\sum_{i=1}^{d} p_i + d - 1\big) + \alpha\big(S_{d+1}(p_1, \ldots, p_d)\big) + \sum_{i=1}^{p_1+\ldots+p_d} D_1\big(v_i|S_{d+1}(p_1, \ldots, p_d)\big),$$

where v_i, $1 \leq i \leq \sum_{i=1}^{d} p_i$, is a terminal vertex of $S_{d+1}(p_1, p_2, \ldots, p_d)$. By a simple calculation we obtain

$$TW\big(S_{d+1}(p_1, \ldots, p_d)\big) = 2(\sum_{i=1}^{d} p_i)^2 - \sum_{i=1}^{d} p_i^2 - \sum_{i=1}^{d} p_i,$$

$$\alpha\big(S_{d+1}(p_1,\ldots,p_d)\big) = \sum_{i=1}^{d}\big[p_i\times 1+3(\sum_{j=1}^{d}p_j-p_i)\big]+2\sum_{i=1}^{d}p_i = 3d\sum_{i=1}^{d}p_i,$$

$$\sum_{i=1}^{p_1+\ldots+p_d} D_1\big(v_i|S_{d+1}(p_1,\ldots,p_d)\big) = \sum_{i=1}^{d}p_i\big[0+p_i\times 1+2(d-1)+3(\sum_{j=1}^{d}p_j-p_i)\big]$$

$$= 3(\sum_{i=1}^{d}p_i)^2-2\sum_{i=1}^{d}p_i^2+2(d-1)\sum_{i=1}^{d}p_i.$$

Substituting the above relations and the formula for $W_{ve_1}\big(S_{d+1}(p_1,p_2,\ldots,p_d)\big)$ given in Theorem 4.1 in (10) and simplifying the resulting expression, we can get (8). To prove (9), note that the Kragujevac tree $Kg(p_1,p_2,\ldots,p_d)$ is a bipartite graph with $2\sum_{i=1}^{d}p_i+d+1$ vertices and $2\sum_{i=1}^{d}p_i+d$ edges. So, by Theorem 2.1,

$$W_{ve_2}\big(Kg(p_1,p_2,\ldots,p_d)\big) = W_{ve_1}\big(Kg(p_1,p_2,\ldots,p_d)\big)+(2\sum_{i=1}^{d}p_i+d+1)(2\sum_{i=1}^{d}p_i+d).$$

Now using (8) and simplifying the resulting expression, we can get (9). □

4.3 Dendrimers

Let D_0 be the graph depicted in Figure 4.

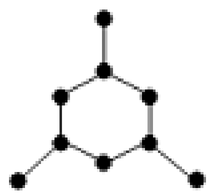

Figure 4: The graph D_0.

For positive integers p and h, let $D_{p,h}$ be a series of dendrimers obtained by attaching p pendent vertices to each pendent vertex of $D_{p,h-1}$ and let $D_{p,0}=D_0$. The dendrimer graph $D_{p,h}$ can also be introduced as the thorn graph obtained by attaching p pendent vertices to each pendent vertex of $D_{p,h-1}$. This molecular structure can be encountered in real chemistry, e.g. in some tertiary phosphine dendrimers. Some examples of this kind of dendrimers are shown in Figure 5. For a fixed positive integer p, let k_h denote the number of pendent vertices of $D_{p,h}$, $h\geq 0$. Obviously, $k_h=pk_{h-1}$ and $|V(D_{p,h})|=|V(D_{p,h-1})|+3p^h$. So for every $h\geq 0$, we have

$$k_h=3p^h,\quad |V(D_{p,h})|=6+3\sum_{i=0}^{h}p^i.$$

Note that, since $D_{p,h}$ is a unicyclic graph, $|E(D_{p,h})|=|V(D_{p,h})|=6+3\sum_{i=0}^{h}p^i$. In [3], an exact formula for computing the terminal Wiener index of the dendrimer graph $D_{p,h}$ was computed.

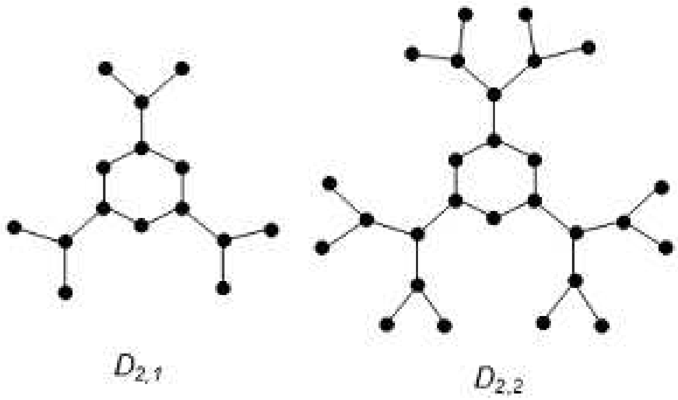

Figure 5: The dendrimer graphs $D_{p,h}$, for $p = 2$ and $h = 1, 2$.

Theorem 4.3 ([3]). *Let p be a positive and h be a nonnegative integer. The terminal Wiener index of the dendrimer graph $D_{p,h}$ is given by*

$$TW(D_{p,h}) = (9h + 12)p^{2h} - 3p^h \sum_{i=0}^{h-1} p^i. \tag{11}$$

In [3], the authors also obtained an exact formula for $D_1(v_h|D_{p,h})$, where v_h is an arbitrary pendent vertex of $D_{p,h}$.

Lemma 4.4 ([3]). *Let p be a positive integer. For every nonnegative integer h, let v_h be an arbitrary pendent vertex of $D_{p,h}$. Then*

$$D_1(v_h|D_{p,h}) = 5 \sum_{k=1}^{h} kp^k + (h + 5) \sum_{k=1}^{h} p^k + 8h + 18. \tag{12}$$

It is easy to check that $\alpha(D_0) = 45$. As a direct consequence of Corollary 3.3, we can obtain a recurrence relation for computing $\alpha(D_{p,h})$.

Corollary 4.5. *Let p and h be nonnegative integers. Then*

$$\alpha(D_{p,h}) = 2pTW(D_{p,h-1}) + p\alpha(D_{p,h-1}) + 3p^h(6 + 3 \sum_{i=0}^{h-1} p^i). \tag{13}$$

Proof. By setting $G = D_{p,h-1}$, $G_P = D_{p,h}$, $k = k_{h-1} = 3p^{h-1}$, and $n = 6+3\sum_{i=0}^{h-1} p^i$ in (3), we can get (13). □

It is easy to check that, $W_{ve_1}(D_0) = 117$. In the following theorem, we present a recurrence relation for computing $W_{ve_1}(D_{p,h})$. Result is easily deduced from (4), and the proof of the theorem is therefore omitted.

THEOREM 4.6. *Let p and h be positive integers. The first vertex-edge Wiener index of the dendrimer graph $D_{p,h}$ is given by*

$$W_{ve_1}(D_{p,h}) = W_{ve_1}(D_{p,h-1}) + 2p(p+1)TW(D_{p,h-1}) + p\alpha(D_{p,h-1}) + 3p^h D_1(v_{h-1}|D_{p,h-1}) + 3p^h(5 + 3\sum_{i=0}^{h} p^i). \quad (14)$$

Since the dendrimer graph $D_{p,h}$ is a bipartite unicyclic graph, by Theorem 2.1 we easily arrive at:

THEOREM 4.7. *Let p be a positive and h be a nonnegative integer. The second vertex-edge Wiener index of the dendrimer graph $D_{p,h}$ is given by*

$$W_{ve_2}(D_{p,h}) = W_{ve_1}(D_{p,h}) + (6 + 3\sum_{i=0}^{h} p^i)^2. \quad (15)$$

Using (11)–(15), we can compute the first and second vertex-edge Wiener indices of the dendrimer graph $D_{p,h}$ for every positive integers p and h.

For example, by (11)–(13), $TW(D_0) = 12$, $D_1(v_0|D_0) = 18$, and $\alpha(D_0) = 45$. Now, by setting $h = 1$ in (14), (15), we get

$$W_{ve_1}(D_{p,1}) = W_{ve_1}(D_0) + 2p(p+1)TW(D_0) + p\alpha(D_0) + 3pD_1(v_0|D_0) + 3p(5 + 3\sum_{i=0}^{1} p^i) = 33p^2 + 147p + 117,$$

$$W_{ve_2}(D_{p,1}) = 42p^2 + 201p + 198.$$

By (11)-(13), $TW(D_{p,1}) = 21p^2 - 3p$, $D_1(v_1|D_{p,1}) = 11p + 26$, and $\alpha(D_{p,1}) = 96p$. Now, by setting $h = 2$ in (14), (15), we get

$$W_{ve_1}(D_{p,2}) = W_{ve_1}(D_{p,1}) + 2p(p+1)TW(D_{p,1}) + p\alpha(D_{p,1}) + 3p^2 D_1(v_1|D_{p,1}) + 3p^2(5 + 3\sum_{i=0}^{2} p^i) = 51p^4 + 78p^3 + 215p^2 + 147p + 117,$$

$$W_{ve_2}(D_{p,2}) = 60p^4 + 96p^3 + 278p^2 + 201p + 198.$$

By (11)-(13), $TW(D_{p,2}) = 30p^4 - 3p^3 - 3p^2$, $D_1(v_2|D_{p,2}) = 17p^2 + 12p + 34$, and $\alpha(D_{p,2}) = 51p^3 + 117p^2$. Now, by setting $h = 3$ in (14), (15), we get

$$W_{ve_1}(D_{p,3}) = W_{ve_1}(D_{p,2}) + 2p(p+1)TW(D_{p,2}) + p\alpha(D_{p,2}) + 3p^3 D_1(v_2|D_{p,2}) + 3p^3(5 + 3\sum_{i=0}^{3} p^i) = 69p^6 + 114p^5 + 135p^4 + 315p^3 + 215p^2 + 147p + 117,$$

$$W_{ve_2}(D_{p,3}) = 78p^6 + 132p^5 + 162p^4 + 387p^3 + 278p^2 + 201p + 198.$$

By (11)–(13), $TW(D_{p,3}) = 39p^6 - 3p^5 - 3p^4 - 3p^3$, $D_1(v_3|D_{p,3}) = 23p^3 + 18p^2 + 13p + 42$, and $\alpha(D_{p,3}) = 69p^5 + 54p^4 + 138p^3$. Now, by setting $h = 4$ in (14), (15), we get

$$W_{ve_1}(D_{p,4}) = W_{ve_1}(D_{p,3}) + 2p(p+1)TW(D_{p,3})$$

$$+ p\alpha(D_{p,3}) + 3p^4 D_1(v_3|D_{p,3}) + 3p^4(5 + 3\sum_{i=0}^{4} p^i)$$
$$= 108p^8 + 165p^7 + 204p^6 + 219p^5 + 417p^4 + 315p^3 + 215p^2 + 147p + 117,$$
$$W_{ve_2}(D_{p,4}) = 117p^8 + 183p^7 + 231p^6 + 255p^5 + 498p^4 + 387p^3 + 278p^2 + 201p + 198.$$

The first and second vertex-edge Wiener indices of $D_{p,h}$ for $p = 2, 3$ and $h \leq 4$ are collected in Tables 1 and 2.

Table 1: The first and second vertex-edge Wiener indices of $D_{2,h}$ for $h \leq 4$.

h	$W_{ve_1}(D_{2,h})$	$W_{ve_2}(D_{2,h})$
0	117	198
1	543	768
2	2711	3440
3	14015	16616
4	79295	89096

Table 2: The first and second vertex-edge Wiener indices of $D_{3,h}$ for $h \leq 4$.

h	$W_{ve_1}(D_{3,h})$	$W_{ve_2}(D_{3,h})$
0	117	198
1	855	1179
2	8730	10755
3	99936	115812
4	1316151	1452312

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