

Distance Degree Index of Some Derived Graphs

Jianzhong Xu ¹, Jia-Bao Liu ^{2*}, Ahsan Bilal ³, Uzma Ahmad ³, Hafiz Muhammad Afzal Siddiqui ^{4*}, Bahadur Ali ³ and Muhammad Reza Farahani ⁵

¹ Department of Electronics and Information Engineering, Bozhou University, Bozhou 236800, China; xujianzhongok@163.com

² School of Mathematics and Physics, Anhui Jianzhu University, Hefei 230601, China

³ Department of Mathematics, University of the Punjab, Lahore 54590, Pakistan; ahsanbilal06@gmail.com (A.B.); uzma.math@pu.edu.pk (U.A.); bahadurali65math@gmail.com (B.A.)

⁴ Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore 54590, Pakistan

⁵ Department of Applied Mathematics, Iran University of Science and Technology, Narmak, Tehran 16844, Iran; Mrfarahani88@gmail.com

* Correspondence: liujiabaoad@163.com (J.-B.L.); hmasiddiqui@gmail.com (H.M.A.S.)

Received: 21 January 2019; Accepted: 14 March 2019; Published: 19 March 2019

Abstract: Topological indices are numerical values associated with a graph (structure) that can predict many physical, chemical, and pharmacological properties of organic molecules and chemical compounds. The distance degree (*DD*) index was introduced by Dobrynin and Kochetova in 1994 for characterizing alkanes by an integer. In this paper, we have determined expressions for a *DD* index of some derived graphs in terms of the parameters of the parent graph. Specifically, we establish expressions for the *DD* index of a line graph, subdivision graph, vertex-semi-total graph, edge-semi-total graph, total graph, and paraline graph.

Keywords: *DD* index; Wiener index; Edge Wiener; degree of a vertex; distance between two vertices

2010 Subject Classification Number: 05C10, 05C12, 05C76

1. Introduction

Graph theory is becoming interestingly significant as it is being actively applied in biochemistry, nanotechnology, electrical engineering, computer science, and operations research [1–4]. The powerful combinatorial method found in graph theory has also been used to prove the results of pure mathematics. A topological index, also known as a graph descriptor, is a real number associated with a graph. Topological indices are helpful for predicting certain physical, chemical, and pharmacological properties of organic molecules and chemical compounds.

A molecular graph is a graphical description of the structural formula of a chemical compound with the help of graph theory. In the construction of a chemical graph, atoms are represented by nodes or vertices and bonds between the atoms are represented by lines or edges [5]. In all major fields of chemistry, chemical graphs are used for many different purposes [6]. As has already been proved in [7], the said indices are useful for characterizing alkanes by an integer. Although the computed expression does not have direct application, we believe that it can be used to compute the said indices for chemical and molecular graphs, which are useful for characterizing alkanes by an integer.

All graphs considered in this paper are simple and connected. Let $G = G(V, E)$ be a simple and connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. The degree of vertex i in G is denoted by $\delta_G(i)$ and is defined as the number of edges incident with vertex i . Also, the degree of an edge $e = ij$ in G is denoted by $\delta_G(e)$ and is defined as the number of edges incident to

both its end vertices, i and j . Mathematically, $\delta_G(e) = \delta_G(i) + \delta_G(j) - 2$. A complete graph on n vertices is denoted by K_n and defined as a graph in which every vertex is adjacent to all other vertices. Let H and K be two subgraphs of G , such that $V(H) \cap V(K) = \emptyset$. Let $i \in V(H)$ and $j \in V(K)$ be the vertices such that

$$d_G(i, j) = \min\{d_G(u, v) : u \in V(H), v \in V(K)\};$$

then i and j are called the terminal vertices of subgraphs H and K in G , as shown in the following figure.

In Figure 1, H and K are subgraphs of graph G . In graph G , the distance between vertex c of H and the vertex f of K is 1, which is the minimum of all vertices of H and K . So, c and f are known as terminal vertices of H and K in G .

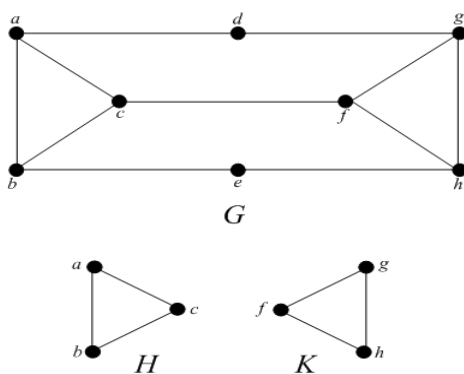


Figure 1. Graph G with its subgraphs H and K .

The first and second Zagreb indices were defined by Gutman and Trinajasti c' in 1972 [8] and very useful in QSPR and QSAR [9–11]. The first and second Zagreb index are defined as:

$$M_1 = M_1(G) = \sum_{ij \in E(G)} [\delta_G(i) + \delta_G(j)] = \sum_{i \in V(G)} \delta_G(i)^2$$

and

$$M_2 = M_2(G) = \sum_{ij \in E(G)} \delta_G(i)\delta_G(j).$$

Another vertex-degree based topological index was found to be useful in the earliest work on Zagreb indices [8], but later it was totally ignored. Quite recently, some interest was shown in it [12,13]. It is called the Forgotten index or simply F-index and defined as:

$$F = F(G) = \sum_{i \in V(G)} \delta_G(i)^3 = \sum_{ij \in E(G)} [\delta_G(i)^2 + \delta_G(j)^2].$$

In 2008, Došli c' introduced the first Zagreb coindex [14], which is defined as:

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{ij \notin E(G)} [\delta_G(i) + \delta_G(j)].$$

In 1947, the chemist Harold Wiener introduced the Wiener index [15], which correlates to the boiling point and structure of the molecule of paraffins. The Wiener index is the oldest topological index and is defined as:

$$W(G) = \sum_{\{i,j\} \subseteq V(G)} d_G(i, j),$$

where $d_G(i, j)$ is the distance in G between the vertices i and j . The Wiener index attracts many chemists and mathematicians and has a long history in the literature. For details, see [16–21]. For the applications of the molecular structures, see [22].

The edge version of the Wiener index was introduced in 2010 [23], and is defined as:

$$W_e(G) = \sum_{\{e,f\} \subseteq E(G)} [d_G(e, f) + 1],$$

where $d_G(e, f)$ is the distance between the edges $e = xy$ and $f = ij$ in G and defined as:

$$d_G(e, f) = \min\{d_G(x, i), d_G(x, j), d_G(y, i), d_G(y, j)\}.$$

The degree distance index (DD index) was introduced in [7] by Dobrynin and Kochetova and is defined as:

$$DD(G) = \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)]d_G(i, j).$$

For a brief look at the different results of DD index, see [24–29]. We define an edge version of DD index as,

$$DD_e(G) = \sum_{\{e,f\} \subseteq E(G)} [\delta_G(e) + \delta_G(f)][d_G(e, f) + 1].$$

The distance between the edge $e = xy$ and a vertex i is defined as

$$d_G(e, i) = \min\{d_G(i, x), d_G(i, y)\}.$$

For basic terminology, see [30].

1.1. Some Derived Graphs

Line Graph: Line graph of a graph G is denoted by $L = L(G)$ such that $V(L) = E(G)$ and there is an edge between two vertices of L if and only if corresponding edges are incident in G . Clearly, $|V(L)| = m$ and by hand shaking-lemma one can easily see that $|E(L)| = \frac{M_1}{2} - m$.

Subdivision Graph: Subdivision graph of a graph G is obtained by inserting a vertex of degree 2 in each edge. Therefore, $|V(S)| = |V(G)| + |E(G)| = n + m$ and $|E(S)| = 2|E(G)| = 2m$.

Vertex-Semitotal Graph: Vertex-Semitotal graph of a graph G is denoted as $T_1 = T_1(G)$ and is obtained by adding a new vertex to each edge of G and then joining a new vertex to the end vertices of the corresponding edge. Thus, $|V(T_1)| = |V(G)| + |E(G)| = n + m$ and

$$|E(T_1)| = |E(S)| + |E(G)| = 2m + m = 3m.$$

Edge-Semitotal Graph: The edge-semitotal graph of a graph G is denoted as $T_2 = T_2(G)$ and is obtained by inserting a new vertex at each edge of G , joining those new vertices by edges whose corresponding edges are incident in G . We have $|V(T_2)| = |E(G)| + |V(G)| = n + m$ and

$$|E(T_2)| = |E(S)| + |E(L)| = m + \frac{M_1}{2}.$$

Total Graph: The union of edge-semitotal graph and vertex-semitotal graph is called total graph of a graph G . It is denoted by $T = T(G)$. Also,

$$|V(T)| = |V(G)| + |E(G)| = n + m \text{ and}$$

$$|E(T)| = |E(G)| + |E(S)| + |E(L)| = 2m + \frac{M_1}{2}.$$

Paraline Graph: The paraline graph $PL = PL(G)$ is the line graph of subdivision graph denoted by $PL = PL(G) = L(S(G))$. Also $|V(PL)| = |E(S)| = 2m$ and

$$|E(PL)| = \frac{M_1(S)}{2} - 2m.$$

In [20], one sees that $M_1(S) = M_1 + 4m$. Thus,

$$|E(PL)| = \frac{M_1 + 4m}{2} - 2m = \frac{M_1}{2}.$$

In Figure 2, self-explanatory examples of these derived graphs are given for a particular graph. In every derived graph of G (except the paraline graph $PL(G)$), the vertices corresponding to the vertices of G are denoted by circles and the vertices corresponding to the edges of G are denoted by squares.

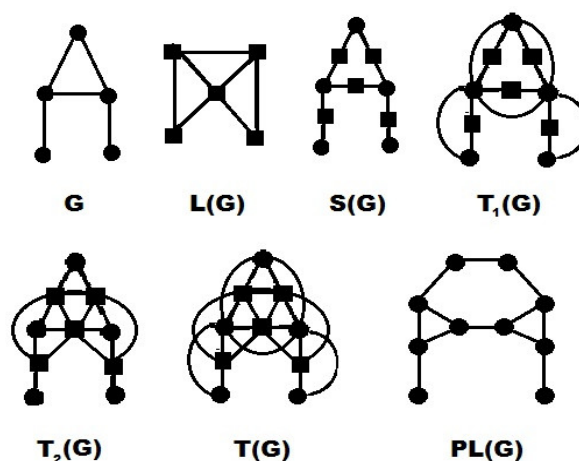


Figure 2. Different graphs derived from G .

The following is a known result of Zagreb indices.

Lemma 1[31] For a graph G with n vertices and m edges, we have

$$\overline{M}_1(G) = 2m(n-1) - M_1(G).$$

1.2. DD Index of Some Derived Graphs

In [31–33] the authors studied the expressions for Zagreb indices and multiplicative Zagreb indices of aforementioned derived graphs. In the past authors dealt only with degree-based indices to derive expressions for the derived graphs. The following proposition encourages us to deal with degree distance-based index. In this section, we study degree distance-based index, DD index for these derived graphs.

Proposition 1 If $L = L(G)$ is line graph of a graph G , then

$$DD(L) = DD_e(G).$$

For a subdivision graph S , a vertex-semi-total graph T_1 , an edge-semi-total graph T_2 , and a total graph T , we can categorize the vertex set into two types of vertices. The first is the set of vertices of G and the second is the set of vertices corresponding to the edges of G . We name them α -type and β -type vertices, respectively. On the basis of this division, there are three types of edges in these graphs:

1. $\alpha\alpha$ -edge, an edge between two α -type vertices,
2. $\beta\beta$ -edge, an edge between two β -type vertices,
3. $\alpha\beta$ -edge, an edge between an α -type vertex and a β -type vertex.

Theorem 1 If $S = S(G)$ is a subdivision graph of graph G , then

$$DD(S) = 2DD(G) + 8W_e(G) + 2m(m+n) + 2 \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 2]d_G(i_\alpha, j_\beta).$$

Proof. We can see that for any α -type vertex i_α of S

$$\delta_S(i_\alpha) = d_G(i_\alpha)$$

and for any β type vertex j_β of S

$$\delta_S(j_\beta) = 2.$$

Also,

$$\begin{aligned} d_S(i_\alpha, j_\alpha) &= 2d_G(i_\alpha, j_\alpha); & i_\alpha, j_\alpha &\in V(G) \\ d_S(i_\beta, j_\beta) &= 2[d_G(i_\beta, j_\beta) + 1]; & i_\beta, j_\beta &\in E(G) \\ d_S(i_\alpha, j_\beta) &= 2d_G(i_\alpha, j_\beta) + 1; & i_\alpha &\in V(G), j_\beta \in E(G). \end{aligned}$$

By definition of the DD index, we have

$$\begin{aligned} DD(S) &= \sum_{\{i,j\} \subseteq V(S)} [\delta_S(i) + \delta_S(j)]d_S(i, j) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(S)} [\delta_S(i_\alpha) + \delta_S(j_\alpha)]d_S(i_\alpha, j_\alpha) + \sum_{\{i_\beta, j_\beta\} \subseteq V(S)} [\delta_S(i_\beta) + \delta_S(j_\beta)]d_S(i_\beta, j_\beta) \\ &\quad + \sum_{\{i_\alpha, j_\beta\} \subseteq V(S)} [\delta_S(i_\alpha) + \delta_S(j_\beta)]d_S(i_\alpha, j_\beta) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)]2d_G(i_\alpha, j_\alpha) + \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [2 + 2]2[d_G(i_\beta, j_\beta) + 1] \\ &\quad + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 2][2d_G(i_\alpha, j_\beta) + 1] \\ &= 2DD(G) + 8W_e(G) + 2m(m+n) + 2 \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 2]d_G(i_\alpha, j_\beta). \end{aligned}$$

Theorem 2 If T_1 is the vertex-semi-total graph of graph G , then

$$DD(T_1) = 2DD(G) + 4W_e(G) + 2m(2m-1+n) + 2 \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 1]d_G(i_\alpha, j_\beta).$$

Proof. First note that for any α -type vertex i_α of T_1

$$d_{T_1}(i_\alpha) = 2d_G(i_\alpha)$$

and for any β -type vertex j_β of T_1

$$d_{T_1}(j_\beta) = 2.$$

Also,

$$d_{T_1}(i_\alpha, j_\alpha) = d_G(i_\alpha, j_\alpha); \quad i_\alpha, j_\alpha \in V(G)$$

$$d_{T_1}(i_\beta, j_\beta) = d_G(i_\beta, j_\beta) + 2; \quad i_\beta, j_\beta \in E(G)$$

$$d_{T_1}(i_\alpha, j_\beta) = d_G(i_\alpha, j_\beta) + 1; \quad i_\alpha \in V(G), j_\beta \in E(G).$$

We have

$$\begin{aligned} DD(T_1) &= \sum_{\{i,j\} \subseteq V(T_1)} [\delta_{T_1}(i) + \delta_{T_1}(j)]d_{T_1}(i, j) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(T_1)} [\delta_{T_1}(i_\alpha) + \delta_{T_1}(j_\alpha)]d_{T_1}(i_\alpha, j_\alpha) \\ &+ \sum_{\{i_\beta, j_\beta\} \subseteq V(T_1)} [\delta_{T_1}(i_\beta) + \delta_{T_1}(j_\beta)]d_{T_1}(i_\beta, j_\beta) \\ &+ \sum_{\{i_\alpha, j_\beta\} \subseteq V(T_1)} [\delta_{T_1}(i_\alpha) + \delta_{T_1}(j_\beta)]d_{T_1}(i_\alpha, j_\beta) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [2\delta_G(i_\alpha) + 2\delta_G(j_\alpha)]d_G(i_\alpha, j_\alpha) + \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [2 + 2][d_G(i_\beta, j_\beta) + 2] \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + 2][d_G(i_\alpha, j_\beta) + 1]. \\ &= 2 \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)]d_G(i_\alpha, j_\alpha) + 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [d_G(i_\beta, j_\beta) + 1] \\ &+ 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} 1 + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + 2]d_G(i_\alpha, j_\beta) \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + 2]. \\ &= 2DD(G) + 4W_e(G) + 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} 1 + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} 2\delta_G(i_\alpha) + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} 2 + 2 \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 1]d_G(i_\alpha, j_\beta). \\ &= 2DD(G) + 4W_e(G) + 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} 1 + 2m(2m) + 2mn + 2 \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 1]d_G(i_\alpha, j_\beta). \end{aligned}$$

Since

$$\sum_{\{i_\beta, j_\beta\} \subseteq E(G)} 1 = \frac{m(m-1)}{2}.$$

Therefore,

$$DD(T_1) = 2DD(G) + 4W_e(G) + 2m(3m-1+n) + 2 \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + 1]d_G(i_\alpha, j_\beta).$$

Theorem 3 If T_2 is an edge-semi-total graph of graph G , then

$$\begin{aligned} DD(T_2) &= DD(G) + DD_e(G) + 4W_e(G) + nM_1(G) \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_{(G)}(i_\alpha, j_\beta). \end{aligned}$$

Proof. To prove this theorem, we proceed in a similar way.

First note that for any α -type vertex i_α of T_2

$$d_{T_2}(i_\alpha) = d_G(i_\alpha)$$

and for any β -type vertex j_β of T_2

$$d_{T_2}(j_\beta) = d_G(j_\beta) + 2.$$

Also, $d_{T_2}(i_\alpha, j_\alpha) = d_G(i_\alpha, j_\alpha) + 1; \quad i_\alpha, j_\alpha \in V(G)$

$$d_{T_2}(i_\beta, j_\beta) = d_G(i_\beta, j_\beta) + 1; \quad i_\beta, j_\beta \in E(G)$$

$$d_{T_2}(i_\alpha, j_\beta) = d_G(i_\alpha, j_\beta) + 1; \quad i_\alpha \in V(G), j_\beta \in E(G).$$

So,

$$\begin{aligned} DD(T_2) &= \sum_{\{i, j\} \subseteq V(T_2)} [\delta_{T_2}(i) + \delta_{T_2}(j)] d_{T_2}(i, j) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(T_2)} [\delta_{T_2}(i_\alpha) + \delta_{T_2}(j_\alpha)] d_{T_2}(i_\alpha, j_\alpha) \\ &+ \sum_{\{i_\beta, j_\beta\} \subseteq V(T_2)} [\delta_{T_2}(i_\beta) + \delta_{T_2}(j_\beta)] d_{T_2}(i_\beta, j_\beta) \\ &+ \sum_{\{i_\alpha, j_\beta\} \subseteq V(T_2)} [\delta_{T_2}(i_\alpha) + \delta_{T_2}(j_\beta)] d_{T_2}(i_\alpha, j_\beta) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)] [d_G(i_\alpha, j_\alpha) + 1] \\ &+ \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [\delta_G(i_\beta) + \delta_G(j_\beta) + 4] [d_G(i_\beta, j_\beta) + 1] \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] [d_G(i_\alpha, j_\beta) + 1]. \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)] d_G(i_\alpha, j_\alpha) + \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)] \\ &+ \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [\delta_G(i_\beta) + \delta_G(j_\beta)] [d_G(i_\beta, j_\beta) + 1] + 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [d_G(i_\beta, j_\beta) + 1] \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] [d_G(i_\alpha, j_\beta)] \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)] d_G(i_\alpha, j_\alpha) + \sum_{i_\alpha, j_\alpha \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)] \\ &+ \sum_{i_\alpha, j_\alpha \notin E(G)} [\delta_G(i_\alpha) + \delta_G(j_\alpha)] + \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [\delta_G(i_\beta) + \delta_G(j_\beta)] [d_G(i_\beta, j_\beta) + 1] \\ &+ 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [d_G(i_\beta, j_\beta) + 1] + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] [d_G(i_\alpha, j_\beta)] \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] \\ DD(T_2) &= DD(G) + M_1(G) + \overline{M}_1(G) + DD_e(G) + 4W_e(G) + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} \delta_G(i_\alpha) + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} \delta_G(j_\beta) + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} 2 + \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] d_G(i_\alpha, j_\beta). \end{aligned}$$

Using the Lemma 1 and relation

$$\sum_{e \in E(G)} \delta_G(e) = \sum_{i \in V(L)} \delta_l(i) = 2 | E(L) | = M_1 - 2m.$$

So,

$$\begin{aligned} DD(T_2) &= DD(G) + M_1(G) + \overline{M_1}(G) + DD_e(G) + 4W_e(G) + m(2m) + n(M_1(G) - 2m) + 2(mn) \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_{(G)}(i_\alpha, j_\beta). \\ DD(T_2) &= DD(G) + DD_e(G) + 4W_e(G) + nM_1(G) \\ &+ 2m[m + n - 1] + \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_{(G)}(i_\alpha, j_\beta). \end{aligned}$$

Theorem 4 If T is the total graph of graph G , then

$$\begin{aligned} DD(T) &= 2DD(G) + DD_e(G) + 4W_e(G) + 4m^2 + nM_1(G) \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_G(i_\alpha, j_\beta) \end{aligned}$$

Proof. First note that for any α -type vertex i_α of T

$$d_T(i_\alpha) = 2d_G(i_\alpha)$$

and for any β -type vertex j_β of T

$$d_T(j_\beta) = d_G(j_\beta) + 2.$$

Also,

$$\begin{aligned} d_T(i_\alpha, j_\alpha) &= d_G(i_\alpha, j_\alpha); & i_\alpha, j_\alpha &\in V(G) \\ d_T(i_\beta, j_\beta) &= d_G(i_\beta, j_\beta) + 1; & i_\beta, j_\beta &\in E(G) \\ d_T(i_\alpha, j_\beta) &= d_G(i_\alpha, j_\beta) + 1; & i_\alpha &\in V(G), j_\beta \in E(G). \\ DD(T) &= \sum_{\{i, j\} \subseteq V(T)} [\delta_T(i) + \delta_T(j)]d_T(i, j) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(T)} [\delta_T(i_\alpha) + \delta_T(j_\alpha)]d_T(i_\alpha, j_\alpha) \\ &+ \sum_{\{i_\beta, j_\beta\} \subseteq V(T)} [\delta_T(i_\beta) + \delta_T(j_\beta)]d_T(i_\beta, j_\beta) \\ &+ \sum_{\{i_\alpha, j_\beta\} \subseteq V(T)} [\delta_T(i_\alpha) + \delta_T(j_\beta)]d_T(i_\alpha, j_\beta) \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [2\delta_G(i_\alpha) + 2\delta_G(j_\alpha)]d_G(i_\alpha, j_\alpha) \\ &+ \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [\delta_G(i_\beta) + \delta_G(j_\beta) + 4][d_G(i_\beta, j_\beta) + 1] \\ &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + \delta_G(j_\beta) + 2][d_G(i_\alpha, j_\beta) + 1]. \\ &= \sum_{\{i_\alpha, j_\alpha\} \subseteq V(G)} [2\delta_G(i_\alpha) + 2\delta_G(j_\alpha)]d_G(i_\alpha, j_\alpha) \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [\delta_G(i_\beta) + \delta_G(j_\beta)][d_G(i_\beta, j_\beta) + 1] + 4 \sum_{\{i_\beta, j_\beta\} \subseteq E(G)} [d_G(i_\beta, j_\beta) + 1] \\
 &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + \delta_G(j_\beta) + 2] \\
 &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_G(i_\alpha, j_\beta). \\
 &= 2DD(G) + DD_e(G) + 4W_e(G) + 4m^2 + n(M_1 - 2m) + 2mn \\
 &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_G(i_\alpha, j_\beta) \\
 DD(T) &= 2DD(G) + DD_e(G) + 4W_e(G) + 4m^2 + nM_1(G) \\
 &+ \sum_{i_\alpha \in V(G), j_\beta \in E(G)} [2\delta_G(i_\alpha) + \delta_G(j_\beta) + 2]d_G(i_\alpha, j_\beta).
 \end{aligned}$$

Lemma 2 For graph G the following equality holds.

$$\sum_{\{i, j\} \subseteq V(G)} [\delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j)][\delta_G(i) + \delta_G(j)] = M_1(G)(2m - n) - 4m^2 + 2M_1(G) - F(G).$$

Proof. First we calculate

$$\begin{aligned}
 &\sum_{i \in V(G)} \sum_{j \in V(G)} [\delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j)][\delta_G(i) + \delta_G(j)] \\
 &= \sum_{j \in V(G)} [M_1(G)\delta_G(j) + 2m\delta_G(j)^2 - M_1(G) - 4m\delta_G(j) - n\delta_G(j)^2] \\
 &= 2M_1(G)(2m - n) - 8m^2.
 \end{aligned}$$

Now the above calculated expression can be written as follows:

$$\begin{aligned}
 &\sum_{i \in V(G)} \sum_{j \in V(G)} [\delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j)][\delta_G(i) + \delta_G(j)] \\
 &= 2 \sum_{\{i, j\} \subseteq V(G)} [\delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j)][\delta_G(i) + \delta_G(j)] \\
 &+ \sum_{i=j \in V(G)} [\delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j)][\delta_G(i) + \delta_G(j)],
 \end{aligned}$$

which gives us the equation

$$\begin{aligned}
 M_1(G)(2m - n) - 4m^2 &= \sum_{\{i, j\} \subseteq V(G)} [\delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j)][\delta_G(i) + \delta_G(j)] \\
 &+ F(G) - 2M_1(G),
 \end{aligned}$$

which completes the proof. ■

Theorem 5 Let G be a graph having no cycle of even length. If $PL = PL(G)$ is a paraline graph of G , then

$$DD(PL) = M_1(G)(2m - n + 1) - 4m^2 + 2 \sum_{\{i, j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)]\delta_G(i)\delta_G(j)d_G(i, j).$$

Proof. It can be noted that for any vertex $i \in V(G)$ there are $\delta_G(i)$ vertices in PL having the same degree as the vertex i such that all the $\delta_G(i)$ vertices are connected with each other. In fact, $PL(G)$ can be obtained from G by replacing every vertex i by $K_{\delta_G(i)}$.

By definition of the DD index,

$$DD(PL) = \sum_{\{u,v\} \subseteq V(PL)} [\delta_{PL}(u) + \delta_{PL}(v)]d_{PL}(u,v).$$

Now, either u or v belongs to the same $K_{\delta_G(i)}$ or two different $K_{\delta_G(i)}$ values, where $i \in V(G)$. So,

$$DD(PL) = \sum_{u,v \in K_{\delta_G(i)}, i \in V(G)} [\delta_{PL}(u) + \delta_{PL}(v)]d_{PL}(u,v) + \sum_{u \in K_{\delta_G(i)}, v \in K_{\delta_G(j)}, \{i,j\} \subseteq V(G)} [\delta_{PL}(u) + \delta_{PL}(v)]d_{PL}(u,v).$$

Here we discuss the two terms one by one.

- I. In the first term, for any vertex $i \in V(G)$ there are a total of $\frac{\delta_G(i)(\delta_G(i)-1)}{2}$ pairs of vertices in $PL(G)$ of degrees $\delta_G(i)$ and having a distance of 1 between them in the corresponding $K_{\delta_G(i)}$.
- II. Before discussing the second term, it is important to see that there is exactly one shortest path in G between any two different vertices, because G has no cycle of even length. Consequently, there is exactly one shortest path between their corresponding complete graphs in $PL(G)$.

Now, in the second term, for any pair of vertices i and j in G , we have the following cases in corresponding pair of complete graphs $K_{\delta_G(i)}$ and $K_{\delta_G(j)}$ in $PL(G)$:

Case-1: There is exactly one pair of terminal vertices in $K_{\delta_G(i)}$ and $K_{\delta_G(j)}$, having distance $[2d_G(i,j)-1]$ between them.

Case-2: There are $[\delta_G(i)-1][\delta_G(j)-1]$ pairs of non-terminal vertices in $K_{\delta_G(i)}$ and $K_{\delta_G(j)}$, having distance $[2d_G(i,j)+1]$ between them.

Case-3: There are $(\delta_G(i)-1)$ pairs of vertices having a non-terminal vertex in $K_{\delta_G(i)}$ and a terminal vertex in $K_{\delta_G(j)}$, and having distance $2d_G(i,j)$ between them. Similarly, there are $(\delta_G(j)-1)$ pairs of vertices having a terminal vertex in $K_{\delta_G(i)}$ and a non-terminal vertex in $K_{\delta_G(j)}$, and having distance $2d_G(i,j)$ between them. So we have a total of $[\delta_G(i) + \delta_G(j) - 2]$ such pairs.

Thus, in light of the above discussion, we have

$$DD(PL) = \sum_{i \in V(G)} \frac{\delta_G(i)(\delta_G(i)-1)}{2} [\delta_G(i) + \delta_G(i)](1) + \sum_{\{i,j\} \subseteq V(G)} (1)[\delta_G(i) + \delta_G(j)][2d_G(i,j)-1] + \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i)-1][\delta_G(j)-1][\delta_G(i) + \delta_G(j)][2d_G(i,j)+1] + \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j) - 2][\delta_G(i) + \delta_G(j)][2d_G(i,j)] = \sum_{i \in V(G)} [\delta_G(i)^3 - \delta_G(i)^2] + \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)][-1 + 2d_G(i,j)] + \delta_G(i)\delta_G(j) - \delta_G(i) - \delta_G(j) + 1 + 2\delta_G(i)\delta_G(j)d_G(i,j) - 2\delta_G(i)d_G(i,j)$$

$$\begin{aligned}
& -2\delta_G(j)d_G(i,j) + 2d_G(i,j) + 2\delta_G(i)d_G(i,j) + 2\delta_G(j)d_G(i,j) - 4d_G(i,j)] \\
& = \sum_{i \in V(G)} [\delta_G(i)^3 - \delta_G(i)^2] \\
& + \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)][-\delta_G(i) - \delta_G(j) + \delta_G(i)\delta_G(j)] \\
& + 2 \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)]\delta_G(i)\delta_G(j)d_G(i,j)
\end{aligned}$$

By using Lemma2, we have

$$\begin{aligned}
DD(PL) &= F - M_1(G) + M_1(G)(2m - n) - 4m^2 - F + 2M_1(G) \\
& + 2 \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)]\delta_G(i)\delta_G(j)d_G(i,j) \\
& = M_1(G)(2m - n + 1) - 4m^2 + 2 \sum_{\{i,j\} \subseteq V(G)} [\delta_G(i) + \delta_G(j)]\delta_G(i)\delta_G(j)d_G(i,j).
\end{aligned}$$

2. Conclusions

In this paper, we studied the DD index of derived graphs, which involves distance and degrees. We computed the expressions to find the DD index of the derived graph by using the parent graph. More specifically, we found the expressions of the DD index using some topological indices of the parent graph. As has already been proved, the said indices are useful for characterizing alkanes by an integer. Although the computed expression does not have direct application, we believe that it can be used to compute the said indices for chemical and molecular graphs, which are useful for characterizing alkanes by an integer.

Author Contributions: These authors contributed equally to this work.

Funding: This work was supported by the Teaching Groups in Anhui Province (2016jytd080, 2015jytd048); the Natural Science Foundation of the Education Department of Anhui Province (KJ2017A704), the Key Program of the Excellent Young Talents Support of Higher Education in Anhui Province (gxyq2018116); the Natural Science Foundation of Bozhou University (BYZ2018B03).

Acknowledgments: Authors are thankful to the referees for their valuable comments to improve this paper.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Tadic, B.; Ziuukovic, J. The graph theory frame work for odeling nano scale systems. *Nanoscale Syst. MMTA* **2013**, *2*, 30–48.
2. Balaban, A.T. Applications of graph theory in chemistry. *J. Chem. Inf. Comput. Sci* **1985**, *25*, 334–343.
3. Abdullahi, S. Anapplication of graph theory to the electrical circuit using matrix method. *J. Math.* **2014**, 164–166, doi:10.9790/5728-1022164166.
4. Shirinivas, S.G.; Vetrivel, S.; Elango, N.M. Applications of graph theory in computer science an overview. *J. Eng. Technol.* **2010**, *2*, 4610–4621.
5. Gold, V.; Loening, K.L.; McNaught, A.D.; Shemi, P. *Compendium of Chemical Terminology*; Blackwell Science Oxford: Oxford, UK, 1997; Volume 1669.
6. Bonchev, D.; Rouvray, D.H. *Chemical Graph Theory Introductions and Fundamentals*; CRC Press: Boca Raton, FL, USA, 1991; Volume 1.
7. Dobrynin, A.A.; Kochetova, A.A. Degree distance of a graph: A degree analogue of the Wiener index. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1082–1086.
8. Gutman, I.; Trinajstić, N. Graph theory and molecular orbitals III. *Total Electron Energy Altern. Hydrocarb. Chem. Phys. Lett.* **1972**, *17*, 535–538.
9. Balaban, A.T. *From Chemical Topology to Three-Dimensional Geometry*; Plenum Press: New York, NY, USA, 1997.

10. Devillers, J.; Balaban, A.T. (Eds.) *Topological Indices and Related Descriptors in QSAR and QSPR*; Gordon and Breach: Amsterdam, The Netherlands, 1999.
11. Todeschini, R.; Consonni, V. *Handbook of Molecular Descriptors*; Wiley-VCH: Weinheim, Germany, 2000.
12. Furtula, B.; Gutman, I. A forgotten topological index. *J. Math. Chem.* **2015**, *53*, 1184–1190.
13. De, N.; Nayeem, S.M.A.; Pal, A. The F-coindex of some graph operations. *Springer Plus* **2016**, *5*, 221.
14. Došlic, T. Vertex-weighted Wiener polynomials for composite graphs. *Ars Math. Contemp.* **2008**, *1*, 66–80.
15. Wiener, H. Structural determination of Paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17–20.
16. Ashrafi, A.R.; Yousafi, S. An exact expression for the Wiener index of a polyhex nanotorus. *MATCH Commun. Math. Comput. Chem.* **2006**, *56*, 169–178.
17. Ashrafi, A.R.; Yousafi, S. A new algorithm for computing distance matrix and Wiener index of zig-zag polyhex nano-tubes, nano-scale. *Res. Lett.* **2007**, *2*, 202–206.
18. Chepoi, V.; Klavzar, S. The Wiener index and the Szeged index of benzoid systems in linear time. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 752–755.
19. Cai, X.; Zhou, B. Reverse Wiener index of connected graphs, *MATCH Commun. Math. Comput. Chem.* **2008**, *60*, 95–105.
20. Dobrynin, A.A.; Entringer, R.; Gutman, I. Wiener index of trees, Theory and applications. *Acta App. Math.* **2011**, *66*, 211–249.
21. Dobrynin, A.A.; Gutman, I.; Klavzar, S.; Zigerl, P. Wiener index of hexagonal systems. *Acta Appl. Math.* **2001**, *72*, 247–294.
22. Sandberg, T.O.; Weinberger, C.; Smått, J.H. Molecular dynamics on wood-derived lignans analyzed by intermolecular network theory. *Molecules* **2018**, *23*, 1990.
23. Iranmanesh, A.; Gutman, I.; Khormali, O.; Mahmiani, A. The edge versions of Wiener index. *Match Commun. Math. Comput. Chem.* **2009**, *61*, 663–672.
24. Ali, P.; Mukwembi, S.; Munyria, S. Degree distance and vertex connectivity. *Disc. Appl. Math.* **2013**, *161*, 2802–2811.
25. Du, Z.; Zhou, B. Degree distance of a graph. *Filomat* **2010**, *24*, 95–120.
26. Ilic, A.; Stevanovic, D.; Feng, L.; Yu, G.; Danklemann, P. Degree distance of unicyclic graphs. *Discr. Appl. Math.* **2011**, *159*, 779–788.
27. Tomescu, I. Unicyclic and bicyclic graphs having minimum degree distance. *Discr. Appl. Math.* **2008**, *156*, 125–130.
28. Tomescu, I. Properties of connected graphs having minimum degree distance. *Discr. Appl. Math.* **2008**, *309*, 2745–2748.
29. Tomescu, I. Ordering connected graphs having small degree distance. *Discr. Appl. Math.* **2010**, *158*, 1714–1717.
30. Bondy, J.A.; Murty, U.S.R. *Graph Theory*; Springer: Berlin, Germany, 2008.
31. Gutman, I.; Furtula, B.; Kovijanic, Z.; Vukicevic; Popivoda, G. On Zagreb indices and coindices. *Match Commun. Math. Comput. Chem.* **2015**, *74*, 5–16.
32. Basavanagoud, B.; Gutman, I.; Gali, C.S. On second Zagreb index and coindex of some derived graphs. *Kragujev. J. Sci.* **2015**, *37*, 113–121.
33. Basavanagoud, B.; Patil, S. Multiplicative Zagreb indices and coindices of some derived graphs. *Opusc. Math.* **2016**, *36*, 287–299.

