A Note on Vertex–Edge Wiener Indices of Graphs

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Received 3 April 2015; Accepted 4 May 2015

ACADEMIC EDITOR: ALI REZA ASHRAFI

ABSTRACT The vertex-edge Wiener index of a simple connected graph G is defined as the sum of distances between vertices and edges of G. Two possible distances $D_1(u,e|G)$ and $D_2(u,e|G)$ between a vertex u and an edge e of G were considered in the literature and according to them, the corresponding vertex-edge Wiener indices $W_{ve_1}(G)$ and $W_{ve_2}(G)$ were introduced. In this paper, we present exact formulas for computing the vertex-edge Wiener indices of two composite graphs named splice and link.

KEYWORDS Distance in graph • vertex–edge Wiener index • Splice • Link.

1. INTRODUCTION

The graphs considered in this paper are undirected, finite and simple. A *topological index* (also known as *graph invariant*) is any function on a graph that does not depend on a labeling of its vertices. The oldest topological index is the one put forward in 1947 by Harold Wiener [1,2] nowadays referred to as the *Wiener index*. Wiener used his index for the calculation of the boiling points of alkanes. The Wiener index $W(G)$ of a connected 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 of G which is defined as the length of any shortest path in G connecting them. Details on the mathematical properties of the Wiener index and its applications in chemistry can be found in [1–8].

In analogy with definition of the Wiener index, the vertex-edge Wiener indices are defined based on distance between vertices and edges of a graph [9,10]. Two possible distances between a vertex u and an edge e=ab of a connected graph G can be considered.

The first distance is denoted by $D_1(u,e|G)$ and defined as [9]:

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

and the second one is denoted by $D_2(u,e|G)$ and defined as [10]:

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

Based on these two distances, two vertex-edge versions of the Wiener index can be introduced. 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 $W_{ve_i}(G) = \sum_{u \in V(G)} \sum_{e \in E(G)} D_i(u, e|G)$, where $i \in \{1,2\}$. It should be explained that, the vertex-edge Wiener index introduced in [9] is half of the first vertex-edge Wiener index W_{ve_1}. However, in the above summation, for every vertex u and edge e of G, the distance $D_i(u, e|G)$ is taken exactly one time into account, so the summation does not need to be multiplied by a half. The first and second vertex-edge Wiener indices are also known as *minimum and maximum indices*, and denoted by $Min(G)$ and $Max(G)$, respectively. Since these indices are considered as the vertex-edge versions of the Wiener index, their present names and notations seem to be more appropriate.

In [10,11], the vertex–edge Wiener indices of some chemical graphs were computed and in [12,13], the behavior of these indices under some graph operations were investigated. In this paper, we present exact formulas for the first and second vertex-edge Wiener indices of two composite graphs named splice and link. Readers interested in more information on computing topological indices of splice and link of graphs, can be referred to [12,14–20].

2. RESULTS AND DISCUSSION

In this section, we compute the first and second vertex–edge Wiener indices of splice and link of graphs. We start by introducing some notations.

Let G be a connected graph. For $u \in V(G)$, we define:

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

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

With the above definitions,

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d(u|G),$$

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

2.1 SPLICE

Let G_1 and G_2 be two connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. For given vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a *splice* [17] of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1.G_2)(a_1, a_2)$ and defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2. We denote by n_i and m_i the order and size of the graph G_i, respectively. It is easy to see that, $|V((G_1.G_2)(a_1, a_2))| = n_1 + n_2 - 1$ and $|E((G_1.G_2)(a_1, a_2))| = m_1 + m_2$.

In the following lemma, the distance between two arbitrary vertices of $(G_1.G_2)(a_1,a_2)$ is computed. The result follows easily from the definition of the splice of graphs, so its proof is omitted.

Lemma 2.1 Let $u,v \in V((G_1.G_2)(a_1,a_2))$. Then

$$d(u,v|(G_1.G_2)(a_1,a_2)) = \begin{cases} d(u,v|G_1) & u,v \in V(G_1) \\ d(u,v|G_2) & u,v \in V(G_2) \\ d(u,a_1|G_1) + d(a_2,v|G_2) & u \in V(G_1),\ v \in V(G_2) \end{cases}.$$

In the following lemma, the distances D_1 and D_2 between vertices and edges of $(G_1.G_2)(a_1,a_2)$ are computed.

Lemma 2.2 Let $u \in V((G_1.G_2)(a_1,a_2))$ and $e \in E((G_1.G_2)(a_1,a_2))$. Then

$$D_i(u,e|(G_1.G_2)(a_1,a_2)) = \begin{cases} D_i(u,e|G_1) & u \in V(G_1),\ e \in E(G_1) \\ D_i(u,e|G_2) & u \in V(G_2),\ e \in E(G_2) \\ d(u,a_1|G_1) + D_i(a_2,e|G_2) & u \in V(G_1),\ e \in E(G_2) \\ d(u,a_2|G_2) + D_i(a_1,e|G_1) & u \in V(G_2),\ e \in E(G_1) \end{cases},$$

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

Proof. Using Lemma 2.1, the proof is obvious. ■

In the following theorem, the first and second vertex-edge Wiener indices of $(G_1.G_2)(a_1,a_2)$ are computed.

Theorem 2.3 The first and second vertex-edge Wiener indices of $G=(G_1.G_2)(a_1,a_2)$ are given by:

$$W_{ve_i}(G) = W_{ve_i}(G_1) + W_{ve_i}(G_2) + m_2 d(a_1|G_1) + m_1 d(a_2|G_2)$$
$$+ (n_2-1)D_i(a_1|G_1) + (n_1-1)D_i(a_2|G_2),$$

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

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

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

Now, we partition the above sum into four sums as follows:

The first sum S_1 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and edges from $E(G_1)$. Using Lemma 2.2, we obtain:

$$S_1 = \sum_{u\in V(G_1)} \sum_{e\in E(G_1)} D_i(u,e|G) = \sum_{u\in V(G_1)} \sum_{e\in E(G_1)} D_i(u,e|G_1) = W_{ve_i}(G_1).$$

The second sum S_2 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and edges from $E(G_2)$. Similar to the previous case, we obtain:

$$S_2 = \sum_{u\in V(G_2)} \sum_{e\in E(G_2)} D_i(u,e|G_2) = W_{ve_i}(G_2).$$

The third sum S_3 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)\setminus\{a_1\}$ and edges from $E(G_2)$. Using Lemma 2.2, we obtain:

$$S_3 = \sum_{u\in V(G_1)\setminus\{a_1\}} \sum_{e\in E(G_2)} D_i(u,e|G) = \sum_{u\in V(G_1)\setminus\{a_1\}} \sum_{e\in E(G_2)} [d(u,a_1|G_1) + D_i(a_2,e|G_2)]$$
$$= m_2 d(a_1|G_1) + (n_1-1) D_i(a_2|G_2).$$

The last sum S_4 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)\setminus\{a_2\}$ and edges from $E(G_1)$. Similar to the previous case, we obtain:

$$S_4 = \sum_{u\in V(G_2)\setminus\{a_2\}} \sum_{e\in E(G_1)} [d(u,a_2|G_2) + D_i(a_1,e|G_1)]$$
$$= m_1 d(a_2|G_2) + (n_2-1) D_i(a_1|G_1).$$

Now the formula of $W_{ve_i}(G)$, $i\in\{1,2\}$, is obtained by adding the quantities S_1, S_2, S_3 and S_4. ■

2.2 LINK

Let G_1 and G_2 be two connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$, respectively. For vertices $a_1\in V(G_1)$ and $a_2\in V(G_2)$, a *link* [17] of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1\sim G_2)(a_1,a_2)$ and obtained by joining a_1 and a_2 by an edge in the union of these graphs. We denote by n_i and m_i the order and size of the graph G_i, respectively. It is easy to see that, $|V((G_1\sim G_2)(a_1,a_2))| = n_1+n_2$ and $|E((G_1\sim G_2)(a_1,a_2))| = m_1+m_2+1$.

In the following lemma, the distance between two arbitrary vertices of $(G_1\sim G_2)(a_1,a_2)$ is computed. The result follows easily from the definition of the link of graphs, so its proof is omitted.

Lemma 2.4 Let $u,v\in V((G_1\sim G_2)(a_1,a_2))$. Then

$$d(u,v|(G_1\sim G_2)(a_1,a_2)) = \begin{cases} d(u,v|G_1) & u,v\in V(G_1) \\ d(u,v|G_2) & u,v\in V(G_2) \\ d(u,a_1|G_1) + d(a_2,v|G_2) + 1 & u\in V(G_1),\ v\in V(G_2) \end{cases}.$$

In the following lemma, the distances D_1 and D_2 between vertices and edges of $(G_1\sim G_2)(a_1,a_2)$ are computed.

Lemma 2.5 Let $u\in V((G_1\sim G_2)(a_1,a_2))$ and $e\in E((G_1\sim G_2)(a_1,a_2))$. Then

$$D_i(u,e|(G_1 \sim G_2)(a_1,a_2)) = \begin{cases} D_i(u,e|G_1) & u \in V(G_1),\ e \in E(G_1) \\ D_i(u,e|G_2) & u \in V(G_2),\ e \in E(G_2) \\ d(u,a_1|G_1) + D_i(a_2,e|G_2) + 1 & u \in V(G_1),\ e \in E(G_2) \\ d(u,a_2|G_2) + D_i(a_1,e|G_1) + 1 & u \in V(G_2),\ e \in E(G_1) \\ d(u,a_1|G_1) + i - 1 & u \in V(G_1),\ e = a_1a_2 \\ d(u,a_2|G_2) + i - 1 & u \in V(G_2),\ e = a_1a_2 \end{cases},$$

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

Proof. Using Lemma 2.4, the proof is obvious. ■

In the following theorem, the first and second vertex-edge Wiener indices of $(G_1 \sim G_2)(a_1,a_2)$ are computed.

Theorem 2.6 The first and second vertex-edge Wiener indices of $G = (G_1 \sim G_2)(a_1,a_2)$ are given by:

$$W_{ve_i}(G) = W_{ve_i}(G_1) + W_{ve_i}(G_2) + (m_2+1)d(a_1|G_1) + (m_1+1)d(a_2|G_2)$$
$$+ n_2D_i(a_1|G_1) + n_1D_i(a_2|G_2) + n_1m_2 + n_2m_1 + (n_1+n_2)(i-1),$$

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

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

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

Now, we partition the above sum into six sums as follows:

The first sum S_1 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and edges from $E(G_1)$. Using Lemma 2.5, we obtain:

$$S_1 = \sum_{u\in V(G_1)}\sum_{e\in E(G_1)} D_i(u,e|G) = \sum_{u\in V(G_1)}\sum_{e\in E(G_1)} D_i(u,e|G_1) = W_{ve_i}(G_1).$$

The second sum S_2 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and edges from $E(G_2)$. Similar to the previous case, we obtain:

$$S_2 = \sum_{u\in V(G_2)}\sum_{e\in E(G_2)} D_i(u,e|G_2) = W_{ve_i}(G_2).$$

The third sum S_3 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and edges from $E(G_2)$. Using Lemma 2.5, we obtain:

$$S_3 = \sum_{u\in V(G_1)}\sum_{e\in E(G_2)} D_i(u,e|G) = \sum_{u\in V(G_1)}\sum_{e\in E(G_2)} [d(u,a_1|G_1) + D_i(a_2,e|G_2) + 1]$$
$$= m_2d(a_1|G_1) + n_1D_i(a_2|G_2) + n_1m_2.$$

The fourth sum S_4 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and edges from $E(G_1)$. Similar to the previous case, we obtain:

$$S_4 = \sum_{u \in V(G_2)} \sum_{e \in E(G_1)} [d(u, a_2 | G_2) + D_i(a_1, e | G_1) + 1]$$
$$= m_1 d(a_2 | G_2) + n_2 D_i(a_1 | G_1) + n_2 m_1 .$$

The fifth sum S_5 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_1)$ and the edge a_1a_2 of G. By Lemma 2.5, we obtain:

$$S_5 = \sum_{u \in V(G_1)} \sum_{e = a_1 a_2} D_i(u, e | G) = \begin{cases} \sum_{u \in V(G_1)} d(u, a_1 | G_1) & i = 1 \\ \sum_{u \in V(G_1)} (d(u, a_1 | G_1) + 1) & i = 2 \end{cases}$$
$$= \begin{cases} d(a_1 | G_1) & i = 1 \\ d(a_1 | G_1) + n_1 & i = 2 \end{cases} .$$

The last sum S_6 consists of contributions to $W_{ve_i}(G)$ of vertices from $V(G_2)$ and the edge a_1a_2 of G. Similar to the previous case, we obtain:

$$S_6 = \sum_{u \in V(G_2)} \sum_{e = a_1 a_2} D_i(u, e | G) = \begin{cases} d(a_2 | G_2) & i = 1 \\ d(a_2 | G_2) + n_2 & i = 2 \end{cases} .$$

Now the formula of $W_{ve_i}(G)$, $i \in \{1,2\}$, is obtained by adding the quantities S_1, S_2, S_3, S_4, S_5 and S_6. ■

ACKNOWLEDGMENTS

The author would like to thank the referee for his/her valuable comments.

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