Applications of Some Graph Operations in Computing Some Invariants of Chemical Graphs

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ABSTRACT

In this paper, we first collect the earlier results about some graph operations and then we present applications of these results in working with chemical graphs.

Keywords: Topological index; graph operation; distance–balanced graph; chemical graph.

1. INTRODUCTION

Throughout this paper all graphs considered are finite, simple and connected. The distance $d_G(u,v)$ between the vertices $u$ and $v$ of a graph $G$ is equal to the length of a shortest path that connects $u$ and $v$. Suppose $G$ is a graph with vertex and edge sets $V = V(G)$ and $E = E(G)$, respectively. For an edge $e = ab$ of $G$, let $n_a(e)$ be the number of vertices closer to $a$ than to $b$. In other words, $n_a^G(e) = |\{u \in V(G) | d(u, a) < d(u, b)\}|$. In addition, let $n_b(e)$ be the number of vertices with equal distances to $a$ and $b$, i.e., $n_0^G(e) = |\{u \in V(G) | d(u, a) = d(u, b)\}|$. We also denote the number of edges of $G$ whose distance to the vertex $a$ is smaller than the distance to the vertex $b$ by $m_a(e)$. The Szeged, edge Szeged, revised Szeged, vertex–edge Szeged, vertex Padmakar–Ivan and edge Padmakar–Ivan indices of the graph $G$ are defined as:

\[
\begin{align*}
S_{zv}(G) &= \sum_{e=uv \in E(G)} n_u(e)n_v(e) \quad \text{(see[1])}, \\
S_{ze}(G) &= \sum_{e=uv \in E(G)} m_u(e)m_v(e) \quad \text{(see[2])}, \\
S_{ze*}(G) &= \sum_{e=uv \in E(G)} (n_u(e)+\frac{n_0(e)}{2})(n_v(e)+\frac{n_0(e)}{2}) \quad \text{(see[3])},
\end{align*}
\]

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A graph \( G \) with a specified vertex subset \( U \subseteq V(G) \) is denoted by \( G(U) \). Suppose \( G \) and \( H \) are graphs and \( U \subseteq V(G) \). The generalized hierarchical product, denoted by \( G(U) \cap H \), is the graph with vertex set \( V(G) \times V(H) \) and two vertices \((g, h)\) and \((g', h')\) are adjacent if and only if \( g = g' \in U \) and \( hh' \in E(H) \) or, \( gg' \in E(G) \) and \( h = h' \). This graph operation has been introduced by Barrière et al. [7,8] and it has some applications in computer science. To generalize this graph operation to \( n \) graphs, assume that \( G_i = (V_i, E_i) \) is a graph with vertex set \( V_i \), \( 1 \leq i \leq N \), having a distinguished or root vertex \( 0 \). The hierarchical product \( H = G_N \cap \ldots \cap G_2 \cap G_1 \) is the graph with vertices the \( N \)-tuples \( x_N, \ldots, x_3, x_2, x_1 \), \( x_i \in V_i \), and edges defined by the following adjacencies:

\[
\begin{align*}
    x_N \ldots x_3 x_2 x_1 & \quad \text{if} \quad x_1 y_1 \in E(G_1) , \\
x_N \ldots x_3 y_2 x_1 & \quad \text{if} \quad x_2 y_2 \in E(G_2) \quad \text{and} \quad x_1 = 0 , \\
x_N \ldots x_3 x_2 y_1 & \quad \text{if} \quad x_3 y_3 \in E(G_3) \quad \text{and} \quad x_1 = x_2 = 0 , \\
\vdots & \quad \vdots \quad \vdots \\
x_N \ldots y_N x_2 y_1 & \quad \text{if} \quad x_N y_N \in E(G_N) \quad \text{and} \quad x_1 = x_2 = \ldots = x_{N-1} = 0 .
\end{align*}
\]

We encourage the reader to consult [9] for the mathematical properties of the hierarchical product of graphs.

The Cartesian product \( G \times H \) of the graphs \( G \) and \( H \) has the vertex set \( V(G \times H) = V(G) \times V(H) \) and \((a, x)(b, y)\) is an edge of \( G \times H \) if \( a = b \) and \( xy \in E(H) \), or \( ab \in E(G) \) and \( x = y \), see[10].

The disjunction \( G \lor H \) of graphs \( G \) and \( H \) is the graph with vertex set \( V(G) \times V(H) \) such that \((u_1, v_1)\) is adjacent to \((u_2, v_2)\) whenever \( u_1 u_2 \in E(G) \) or \( v_1 v_2 \in E(H) \) [10].

Let \( G = (V, E) \) be a simple graph of order \( n = |V| \). Given \( u, v \in V \), \( u \sim v \) means that \( u \) and \( v \) are adjacent vertices. Given a set of vertices \( S = \{v_1, v_2, \ldots, v_k\} \) of a connected graph \( G \), the metric representation of a vertex \( v \in V \) with respect to \( S \) is the vector \( r(v|S) = (d_G(v, v_1), d_G(v, v_2), \ldots, d_G(v, v_k)) \). We say that \( S \) is a resolving set for \( G \) if for every pair of distinct vertices \( u, v \in V \), \( r(u|S) \neq r(v|S) \). The metric dimension of \( G \) is the minimum cardinality of any resolving set for \( G \), and it is denoted by \( \text{dim}(G) \).
Now, we present some certain types of graphs that play prominent roles in this work. A graph $G$ is called nontrivial if $|V(G)| > 1$. The $n$-cube $Q_n$ ($n \geq 1$) is the graph whose vertex set is the set of all $n$-tuples of 0s and 1s, where two $n$-tuples are adjacent if they differ in precisely one coordinate. A tree is an undirected graph in which any two vertices are connected by exactly one simple path. In other words, any connected graph without cycles is a tree. A regular graph is a graph where each vertex has the same number of neighbors. A regular graph with vertices of degree $k$ is called a $k$–regular graph or regular graph of degree $k$. Note that the path graph, the complete and the cycle of order $n$ are denoted by $P_n$, $K_n$ and $C_n$, respectively.

2. **Main Results**

In what follows, we assume that $\prod_j f_i = 1$ and $\sum_j f_i = 0$ for each $i, j \in \{0, 1, 2, \ldots\}$, that $i - j = 1$. Furthermore, let $\prod_i f_i = \sum_i f_i = 0$, for every $i, j \in \{0, 1, 2, \ldots\}$, such that $i - j > 1$. For a rooted graph $G$ with root vertex $r$, we will use $\Gamma_v(G)$ to denote the sum of $n^{G}_{v}(e)$ over all edges $e = uv$ of $G$ that $d_G(u, r) < d_G(v, r)$ and $\Gamma^{c}_v(G)$ to denote the sum of $n^{G}_{v}(e)$ over all edges $e = uv$ of $G$ that $d_G(u, r) < d_G(v, r)$. Moreover, $\Gamma^c_\Gamma(G)$ denotes the sum of $m^{G}_{v}(e)$ over all edges $e = uv$ of $G$ that $d_G(u, r) < d_G(v, r)$ and $\Gamma^{c}_e(G)$ denotes the sum of $m^{G}_{v}(e)$ over all edges $e = uv$ of $G$ that $d_G(u, r) < d_G(v, r)$. In other words,

$$\Gamma_\Gamma(G) = \sum_{uv \in E(G), d_G(u, r) < d_G(v, r)} n^{G}_{v}(uv),$$

$$\Gamma^{c}_v(G) = \sum_{uv \in E(G), d_G(u, r) < d_G(v, r)} m^{G}_{v}(uv),$$

$$\Gamma_e(G) = \sum_{uv \in E(G), d_G(u, r) < d_G(v, r)} m^{G}_{v}(uv),$$

$$\Gamma^{c}_e(G) = \sum_{uv \in E(G), d_G(u, r) < d_G(v, r)} m^{G}_{v}(uv).$$

If the vertex $r$ lies on no odd cycle of $G$, then one can easily see that

$$PL_\Gamma(G) = \Gamma_\Gamma(G) + \Gamma^{c}_v(G) \quad \text{and} \quad PL_e(G) = \Gamma_e(G) + \Gamma^{c}_e(G).$$

Also, for a sequence of graphs, $G_1$, $G_2$, ..., $G_n$, we set $|V_{i,j}| = \prod_{k=1}^{j} |V(G_k)|$ and $|V_{i,j}| = \prod_{k=i, k \neq j}^{j} |V(G_k)|$. To say the next result, we have to present some notation. For a connected rooted graph $G$ with root vertex $r$, let $N^{G}(r)$ be the set of vertices of $G$ with the property that $u \in N^{G}(r)$ if there exists $v \neq u$ in $V(G)$ such that $d_G(u, r) = d_G(v, r)$. We say that
$S(N^G(r)) \subseteq V(G)$ is a resolving set for $N_G(r)$ if for each pair of distinct vertices $u, v \in N^G(r)$, $r(u|S(N^G(r))) \neq r(v|S(N^G(r)))$. Therefore, it is clear that $\dim(N^G(r)) \leq \dim(G)$. The metric dimension of $N^G(r)$ is the minimum cardinality of any resolving set for $N^G(r)$, and it is denoted by $\dim(N^G(r))$.

**Theorem 1.** [9]. Suppose $G_1, G_2, \ldots, G_n$ are nontrivial connected rooted graphs with root vertices $r_1, \ldots, r_n$, respectively. Then

$$\dim(G_n \cap \ldots \cap G_2 \cap G_1) = \begin{cases} \prod_{j=2}^{n} |V(G_j)| \dim(N^{G_j}(r_j)) & \text{if } G_j \not\cong P_n \\ \prod_{j=3}^{n} |V(G_j)| \dim(N^{G_j \cup G_j}(r_2)) & \text{if } G_j \cong P_n \end{cases}$$

![Diagram](image-url)

**Figure 1:** Irregular Dicentric $IDD_{5(2,1,3,1,2)}$ Dendrimer.

**Example 2.** Let $IDD_r(p_1,\ldots,p_r)$ be the graph of the irregular dicentric dendrimer that $p_i > 1$, $i=1,\ldots, r$, see [11] for more information. Then $IDD_{r}(p_1,\ldots,p_r) = P_2 \cap H$, where $H$ is a tree of progressive degrees $p_i$, $i=1,\ldots,r$, respectively, and generation $r$ (see Figure 1). One can see that $\dim(N^H(r)) = \prod_{i=1}^{r-1} p_i(p_r - 1)$. Therefore, by Theorem 1, we have:

$$\dim(IDD_{r}(p_1,\ldots,p_r)) = |V(P_2)| \dim(N^H(r)) = 2 \prod_{i=1}^{r-1} p_i(p_r - 1).$$

A graph $G$ is said to be (vertex) distance-balanced, if $n_a^G(e) = n_b^G(e)$, for each edge $e = ab \in E(G)$, see [12, 13] for details. These graphs first studied by Handa [14] who considered distance-balanced partial cubes. In [15], Jerebic et al. studied distance-balanced...
graphs in the framework of various kinds of graph products. After that, in [16], the present authors introduced the concept of edge distance-balanced graphs. Such a graph $G$ has this property that $m^G_a(e) = m^G_b(e)$ holds for each edge $e = ab \in E(G)$.

**Proposition 3.** [13]. Let $G$ and $H$ be arbitrary, nontrivial and connected graphs. Then $G \vee H$ is distance-balanced if and only if $G$ and $H$ are regular graphs.

**Example 4.** Consider $G'$, see Figure 2, that was constructed in [17] as an example of a bipartite regular graph that is not distance-balanced. It would be interesting to know that we can produce a distance-balanced graph by two graphs which are not distance-balanced. Let $G$ is arbitrary, nontrivial and connected regular graph then by the above proposition, $G' \vee G$ is distance-balanced (note that $G$ can be not distance-balanced).

**Theorem 5.** [16]. Let $G$ and $H$ be edge and vertex distance-balanced graphs. Then $G \times H$ is edge distance-balanced graphs.

**Example 6.** Consider the $N$-cube $Q_N$. It is well-known fact that it can be written in the form $Q_N = \times_{i=1}^N K_2$. On the other hand, $K_2$ is edge and vertex distance-balanced graph. So, by the above theorem, $Q_N$ is edge distance-balanced graph.

**Theorem 7.** [18]. Suppose $G_1, G_2, ..., G_n$ are connected rooted graphs with root vertices $r_1, ..., r_n$, respectively. Then

$$S_{z_i}(G_n \wedge ... \wedge G_2 \wedge G_1) = \sum_{i=1}^n v_{i+1,n} \| v_{i,i-1} \|^2 S_{z_i}(G_i)$$
\begin{align*}
&\quad + \sum_{i=1}^{n-l} \left( \sum_{j=i+1}^{n} |V(G_j)| - 1 \right) |V_{i,j-1}| \right) \left| V_{i,n} \right| \Gamma_v(G_i). \\
\textbf{Corollary 8.} \ [18]. \ Suppose \ G_1, \ G_2, \ ... , \ G_n \ are \ connected, \ rooted \ and \ distance-balanced \ graphs \ with \ root \ vertices \ r_1, \ ... , \ r_n, \ respectively, \ such \ that \ r_i \ lies \ on \ no \ odd \ cycle \ of \ G_i, \ i = 1, 2, \ldots, n. \ Then \\
S_{\varepsilon}(G_n \cap \ldots \cap G_2 \cap G_1) = \sum_{i=1}^{n} |V_{i+1,n}| \left| V_{i,i-1} \right| S_{\varepsilon}(G_i) \\
&\quad + \frac{1}{2} \sum_{i=1}^{n-l} \left( \sum_{j=i+1}^{n} |V(G_j)| - 1 \right) |V_{i,j-1}| \right) \left| V_{i,n} \right| \Gamma_v(G_i). \\
\textbf{Theorem 9.} \ [18]. \ Suppose \ G_1, \ G_2, \ ... , \ G_n \ are \ connected \ rooted \ graphs \ with \ root \ vertices \ r_1, \ ... , \ r_n, \ respectively. \ Then \\
S_{\varepsilon}(G_n \cap \ldots \cap G_2 \cap G_1) = \sum_{i=1}^{n} |V_{i+1,n}| \left| S_{\varepsilon}(G_i) \right| \\
&\quad + \sum_{i=1}^{n} |V_{i+1,n}| \left( \sum_{j=1}^{i-l} |E(G_j)| \left| V_{j+1,i-1} \right| \right) S_{\varepsilon}(G_i) \\
&\quad + 2 \sum_{i=1}^{n} |V_{i+1,n}| \left( \sum_{j=1}^{i-l} |E(G_j)| \left| V_{j+1,i-1} \right| \right) S_{\varepsilon}(G_i) \\
&\quad + \sum_{i=1}^{n} |V_{i+1,n}| \left( \Gamma_e(G_i) + \Gamma_v(G_i) \sum_{j=1}^{i-l} |E(G_j)| \left| V_{j+1,i-1} \right| \right) \\
&\quad + \sum_{j=i+1}^{n} \left( |V(G_j)| - 1 \sum_{k=i}^{j-l} |E(G_k)| \left| V_{k+1,j-1} \right| + |E(G_j)| \right). \\
\textbf{Corollary 10.} \ [18]. \ Suppose \ G_1, \ G_2, \ ... , \ G_n \ are \ connected, \ rooted, \ distance-balanced \ and \ edge \ distance-balanced \ graphs \ with \ root \ vertices \ r_1, \ r_2, \ ... , \ r_n, \ respectively, \ such \ that \ r_i \ lies \ on \ no \ odd \ cycle \ of \ G_i, \ i = 1, 2, \ldots, n. \ Then \\
S_{\varepsilon}(G_n \cap \ldots \cap G_2 \cap G_1) = \sum_{i=1}^{n} |V_{i+1,n}| \left| S_{\varepsilon}(G_i) \right|
+ \sum_{i=1}^{n} V_{i+1,n} \left( \sum_{j=1}^{i-1} |E(G_j)| \mid V_{j+1,j-1} \right) - \sum_{i=1}^{n} |V_{i+1,n}| \mid V_{i+1,i-1} \mid |V(G_i)| |E(G_i)| + \sum_{i=1}^{n} \frac{|V_{i+1,n}|}{4} \left( \sum_{j=i+1}^{n} (|V(G_j)| \mid V_{j+1,j-1}^2) \right) N_i + \sum_{i=1}^{n} \frac{|V_{i+1,n}|}{2} \left( \sum_{j=i+1}^{n} (|V(G_j)| \mid V_{j+1,j-1}^2) \right) \pi_v(G_i).

\textbf{Theorem 11.} [18]. Suppose \( G_1, G_2, \ldots, G_n \) are connected rooted graphs with root vertices \( r_1, r_2, \ldots, r_n \), respectively. Then

\[ S_{z_{v}}(G_n \sqcap \ldots \sqcap G_2 \sqcap G_1) = \sum_{i=1}^{n} |V_i| |V_{i+1,n}| \mid V_{i+1,i-1} \mid S_{z_{v}}(G_i) \]

\[ + \sum_{i=1}^{n} \frac{|V_{i+1,n}|}{2} \left( \sum_{j=i+1}^{n} (|V(G_j)| \mid V_{j+1,j-1}^2) \right) |V(G_i)| |E(G_i)| + \sum_{i=1}^{n} \frac{|V_{i+1,n}|}{4} \left( \sum_{j=i+1}^{n} (|V(G_j)| \mid V_{j+1,j-1}^2) \right) N_i + \sum_{i=1}^{n} \frac{|V_{i+1,n}|}{2} \left( \sum_{j=i+1}^{n} (|V(G_j)| \mid V_{j+1,j-1}^2) \right) \pi_v(G_i) \]

where \( N_i = \{|uv \in E(G_i) \mid d_{G_i}(u, r_i) = d_{G_i}(v, r_i)\}|. \)

\textbf{Corollary 12.} [18]. Suppose \( G_1, G_2, \ldots, G_n \) are connected, rooted, bipartite and distance-balanced graphs with root vertices \( r_1, r_2, \ldots, r_n \), respectively. Then

\[ S_{z_{v}}(G_n \sqcap \ldots \sqcap G_2 \sqcap G_1) = \sum_{i=1}^{n} |V_i| |V_{i+1,n}| \mid V_{i+1,i-1} \mid S_{z_{v}}(G_i) \]

\[ + \sum_{i=1}^{n} \frac{|V_{i+1,n}|}{2} \left( \sum_{j=i+1}^{n} (|V(G_j)| \mid V_{j+1,j-1}^2) \right) \pi_v(G_i). \]
Example 13. Octanitrocubane is the most powerful chemical explosive with formula $C_8(NO_2)_8$, Figure 3. Let $H$ be the molecular graph of this molecule. Then obviously $H = Q_3 \ast P_2$. On the other hand, one can easily see that $Sz_v(Q_3) = Sz_e(Q_3) = Sz_{ev}(Q_3) = 192$, $\Gamma_v(P_2) = 1$ and $\Gamma_e(P_2) = 0$ and so, by the above results, we have:

$$Sz_v(H) = Sz_v(Q_3 \ast P_2) = 888, Sz_e(H) = Sz_e(Q_3 \ast P_2) = 768, Sz_{ev}(H) = Sz_{ev}(Q_3 \ast P_2) = 888.$$ 

Example 14. Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $v_i \in V(G_i)$. The bridge–cycle graph $BC(G_1, G_2, ..., G_d) = BC(G_1, G_2, ..., G_d; v_1, v_2, ..., v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs $G_1, ..., G_d$ by connecting the vertices $v_i$ and $v_{i+1}$ by an edge for all $i = 1, 2, ..., d-1$ and connecting the vertices $v_1$ and $v_d$ by an edge, see Figure 4. Suppose that $G_1 = ... = G_d = G$. Then we have $BC(G_1, G_2, ..., G_d) \cong C_d \cap G$. On the other hand, It is not so difficult to check that

$$Sz_v(C_n) = \begin{cases} \frac{n^3}{4} & 2 \nmid n \\
^2(n-1) \quad 2 \mid n 
\end{cases}.$$ 

Therefore, if $2 \mid n$, by Theorem 1, we have $Sz_v(C_n \cap G) = n$. 

**Figure 3:** The Molecular Graph of Octanitrocubane.

**Figure 4:** The Bridge–Cycle Graph.
\[ Sz_v(G) + \frac{n^3}{4} |V(G)|^2 + n(n-1)|V(G)|\Gamma_v(G) \] and if \( 2 \mid n \), then \( Sz_v(C_n \cap G) = n \ Sz_v(G) + \frac{n(n-1)^2}{4} |V(G)|^2 + n(n-1)|V(G)|\Gamma_v(G) \).

By replacing \( G \) with \( P_m \) (such that \( r \) is a pendant vertex of \( P_m \)) in the above relations, we obtain \( Sz_v \) of \( \text{Sun}_n, m-1 \), see [19], as follow:

\[
Sz_v(\text{Sun}_{n,m-1}) = \begin{cases} 
\frac{1}{4} n^3 m^2 + \frac{1}{2} n^2 m^3 - \frac{1}{2} n^2 m^2 - \frac{1}{3} nm^3 + \frac{1}{2} nm^2 - \frac{1}{6} nm & 2 \mid n \\
\frac{1}{4} n^3 m^2 - n^2 m^2 + \frac{3}{4} nm^2 + \frac{1}{2} n^2 m^3 - \frac{1}{3} nm^3 - \frac{1}{6} nm & 2 \nmid n
\end{cases}
\]

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REFERENCES