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DISTANCE ECCENTRIC CONNECTIVITY INDEX OF THE LINE GRAPH OF LINEAR CHAIN OF BENZENE

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Abstract

Distance eccentric connectivity index is a distance-based topological indices that was currently applied to mathematical modeling of various biological functions. This study evaluates the exact results of the distance eccentric connectivity index of the line graph of linear chain of benzene.

1. Introduction

The topological index can study the chemical characteristics of drugs [5]. In the literature, numerous distance based topological indices have been displayed [6] and established some applications in QSPR/QSAR research [2]. All over this paper we apply molecular graph $G = (V, E)$, a connected graph having no parallel edges and no loops where edges and vertices denote to chemical bonds and atoms of the compound. For an individual vertices $v \in V$, the number of edges incident on it is called its degree, $\deg(v)$. The length of the minimum path connecting two vertices u and v of G is the distance $d_G(u, v)$. Another distance based notion is eccentricity which is the farthest distance between a vertex u and all other points in G. The radius and the diameter of a graph are the minimum and maximum eccentricities at all

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vertices denoted by $rad(G)$ and $diam(G)$, respectively. We see [4] for unspecified terms and notation. In 1947, Harary Weiner was first presented one of the oldest distance based index termed as Weiner index. When examining the antihypertensive activity of N-benzylimidazole derivatives, Gupta [3] introduced a new topological descriptor termed as connectivity eccentricity index. Sharma et al. [7] introduced the concept eccentric connectivity index (ECI) $\xi^c(G)$ as $\xi^c(G) = \sum_{v \in V} \deg(v) e(v)$. The first Zagreb eccentricity is defined as $\zeta_1(G) = \sum_{v \in V} (e(v))^2$. In 2021, Alqesmah et al. [1] defined distance eccentric connectivity index (DECI) of G as,

$$\xi^{De}(G) = \sum_{v \in V} \deg^{De}(v) e(v). \tag{1}$$

Where $\deg^{De}(v)$, the distance eccentricity degree of the vertex v in G, which is the cardinality of $N_{De}(v)$. That is,

$$\deg^{De}(v) = |N_{De}(v)| = |\{u \in V : d_G(u, v) = e(u)\}|.$$

The sum of the distances eccentricity degrees of all the vertices of G is denoted by $Q(G)$. The first Zagreb distance eccentricity indices [1] is $M_1^{De}(G) = \sum_{u \in V(G)} (\deg^{De}(u))^2$. The maximum and minimum distance eccentricity degrees [1] over all vertices of G is indicated by $\Delta^{De}(G) = \max_{u \in V(G)} |N_{De}(u)|$ and $\delta^{De}(G) = \max_{u \in V(G)} |N_{De}(u)|$ respectively.

Moreover, the set of vertices with $e(u) = \alpha$ in G by V_e^{α}, $\alpha = 1, 2, 3, \ldots, diam(G)$.

1.1 Linear Chains of Benzene

In the industry of hydrocarbons, benzenoid graphs play a key role which is an organic chemical compound made up of six carbon atoms each attached to one hydrogen atom with the molecular formula C_6H_6. Linear chain of benzene (linear hexagonal chain) composed of a fusion of n benzene rings.

The fusion of 3, 4 benzene rings named as anthracene and tetracene are shown in Figure 1. All over this paper, we represent the linear chain of benzene by Ln.

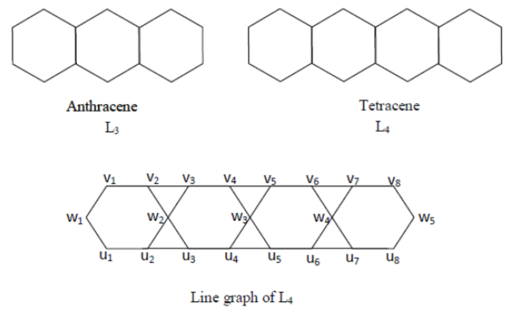

Figure 1. Linear Chain of n Benzene for $n = 3, 4$ and the line graph of L_4.

In this paper, we calculate some results on the DECI for the line graph of L_n. Line graph $L(G)$, is a simple graph whose vertices are edges of G and $e_1e_2 \in E(L(G))$ if, $e_1, e_2 \in E(G)$ have a common terminal (end) vertex in G. Let $G = (L(L_n))$ be the line graph of L_n. The vertices of G have three partitions,

$$|V_2| = |\{u \in V : d_u = 2\}| = 6.$$

$$|V_3| = |\{u \in V : d_u = 3\}| = 4n - 4.$$

$$|V_4| = |\{u \in V : d_u = 4\}| = n - 1.$$

Thus $|V(G)| = |V_2| + |V_3| + |V_4| = [6 + (4n - 4) + (n - 1)] = 5n + 1.$ By Handshaking lemma,

$$|E(G)| = \frac{1}{2}\sum_{u \in V} d_u = \frac{1}{2}[2(6) + 3(4n - 4) + 4(n - 1)] = 8n - 2.$$

Table 1. First and third row vertex partition of $L(L_n)$.

Vertices	Eccentricity	$\deg^{De}(u)$	$\deg(u)$
v_1, u_1, v_{2n}, u_{2n}	$2n$	2	2
$v_2, u_2, v_{2n-1}, u_{2n-1}$	$2n - 1$	2	3

$v_3, u_3, v_{2n-2}, u_{2n-2}$	$2n-2$	2	3
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$v_n, u_n, v_{n+1}, u_{n+1}$	$2n-(n-1)=n+1$	2	3

The authors [1] investigated the distance eccentric connectivity index of path, cycle, wheel, complete graph, complete bipartite and determined general bounds. Here we compute distance eccentric connectivity index of the line graph of linear chains of benzene.

Table 2. Second row vertex partition of $L(L_n)$, for odd n.

Vertices	Eccentricity	$\deg^{De}(u)$	$\deg(u)$
w_1, w_{n+1}	$\left(n+2\left(\left\lfloor\frac{n}{2}\right\rfloor+1\right)\right)$	1	2
w_2, w_n	$\vdots$	1	4
w_3, w_{n-1}	$\vdots$	1	4
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$w_{\left\lfloor\frac{n}{2}\right\rfloor-1}, w_{\left\lfloor\frac{n}{2}\right\rfloor+4}$	$n+2(3)$	1	4
$w_{\left\lfloor\frac{n}{2}\right\rfloor}, w_{\left\lfloor\frac{n}{2}\right\rfloor+3}$	$n+2(2)$	1	4
$w_{\left\lfloor\frac{n}{2}\right\rfloor+1}, w_{\left\lfloor\frac{n}{2}\right\rfloor+2}$	$n+2(1)$	1	4

Table 3. Second row vertex partition of $L(L_n)$, for even n.

Vertices	Eccentricity	$\deg^{De}(u)$	$\deg(u)$
w_1, w_{n+1}	$\left(n+2\left(\left\lfloor\frac{n}{2}\right\rfloor-1\right)\right)$	1	2

w_2, w_n	$\vdots$	1	4
w_3, w_{n-1}	$\vdots$	1	4
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$w_{\frac{n}{2}-1}, w_{\frac{n}{2}+3}$	$n+(2(2)-1)$	1	4
$w_{\frac{n}{2}}, w_{\frac{n}{2}+2}$	$n+(2(1)-1)$	1	4
$w_{\frac{n}{2}+1}$	$n+1$	2	4

2. Main Results

We present the results based on distance eccentricity connectivity index of $L(L_n)$ in this section. Table [1-3] shows the vertex-eccentricity partition of $L(L_n)$.

Theorem 2.1. *Let* $G = L(L_n)$. *Then*

$$\xi^{De}(G) = \begin{cases} \sum_{k=1}^{n} 4[2(2n-(k-1))] + \sum_{k=1}^{\left\lfloor \frac{n}{2} \right\rfloor + 1} 2[(n+2k)] & \text{for } n \geq 3 \\ \sum_{k=1}^{n} 4[2(2n-(k-1))] + \left[\sum_{k=1}^{\frac{n}{2}} 2(n+(2k-2)) \right] + (n+1) & \text{for } n \geq 4. \end{cases}$$

Proof. Let $\{v_i : i = 1, 2, \ldots, 2n\}$ and $\{u_i : i = 1, 2, \ldots, 2n\}$ be the first and third row of vertex sets and let $\{w_i : i = 1, 2, \ldots, n+1\}$ be the second row of vertex set of $L(L_n)$ as in Figure 1. The following cases are discussed by using Table [1-3] respectively.

Case 1. For odd n; $n \geq 3$.

From the figure of $L(L_n)$, there are n sets consists of four vertices namely $\{u_i, v_i / i = 1, 2n\}; \{u_i, v_i / i = 1, 2, \ldots, 2n-1\}, \ldots, \{u_i, v_i / i = n, n+1\}$ have eccentricity $2n, (2n-1), (2n-2), \ldots, (2n-(n-1))$ and $\deg^{De}(u) = 2$ respectively. Again there are $\left(\left\lfloor \frac{n}{2} \right\rfloor + 1\right)$ sets consists of two vertices namely $\{w_i / i = 1, n+1\}, \{w_i / i = 2, n\}, \ldots, \left\{w_i / i = \left\lfloor \frac{n}{2} \right\rfloor - 1, \left\lfloor \frac{n}{2} \right\rfloor + 4\right\}, \left\{w_i : i = \left\lfloor \frac{n}{2} \right\rfloor, \left\lfloor \frac{n}{2} \right\rfloor + 3\right\},$ $\left\{w_i : i = \left\lfloor \frac{n}{2} \right\rfloor + 1, \left\lfloor \frac{n}{2} \right\rfloor + 2\right\}$ have eccentricity $\left(n + 2\left(\left\lfloor \frac{n}{2} \right\rfloor + 1\right)\right), \ldots, (n + 2(3)),$ $(n + 2(2)), (n + 2(1))$ and $\deg^{De}(u) = 1$ respectively. Using Definition (1), we get

$$\xi^{De}(G) = \sum_{k=1}^{n} 4[2(2n - (k-1))] + \sum_{k=1}^{\left\lfloor \frac{n}{2} \right\rfloor + 1} 2[(n + 2k)].$$

Case 2: For even n; $n \geq 4$.

There are n sets consists of four vertices namely $\{ui, vi / i = 1, 2n\}, \{ui, vi / i = 1, 2, \ldots, 2n-1\}, \ldots, \{ui, vi / i = n, n+1\}$ have eccentricity $2n, (2n-1), (2n-2), \ldots, (2n-(n-1))$ and $\deg^{De}(u) = 2$ respectively. Again there are $\left(\frac{n}{2}\right)$ sets consists of two vertices namely $\{w_i / i = 1, n+1\}, \{w_i / i = 2, n\}, \ldots, \left\{w_i : i = \frac{n}{2} - 2, \frac{n}{2} + 4\right\}, \left\{w_i : i = \frac{n}{2} - 1, \frac{n}{2} + 3\right\},$ $\left\{w_i : i = \frac{n}{2}, \frac{n}{2} + 2\right\}$ have eccentricity $\left(n + 2\left(\frac{n}{2} + 1\right)\right), \ldots, (n + (2(3) - 1)),$ $(n + (2(2) - 1)), (n + (2(1) - 1))$ and $\deg^{De}(u) = 1$ respectively, also there is only one set consist of a vertex namely $\left\{w_{\frac{n}{2}+1}\right\}$ have eccentricity $(n+1)$ and $\deg^{De}(u) = 2.$ Using Definition (1), we get

$$\xi^{De}(G) = \sum_{k=1}^{n} 4[2(2n - (k-1))] + \left[\sum_{k=1}^{\frac{n}{2}} 2(n + 2k - 1)\right] + (n+1).$$

Theorem 2.2. *Let* $G = L(L_n)$. *Then*

$$\xi^c(G) = \begin{cases} 4(2(2n)) + \sum_{k=1}^{n} 4[3(2n-k)] + 2(2(2n+1)) + \sum_{k=1}^{\left\lfloor \frac{n}{2} \right\rfloor} 2[4(2n-(2k-1))] & for\ n \geq 3 \\ 4(2(2n)) + \sum_{k=1}^{n} 4[3(2n-k)] + 2(2(2n+1)) + \left[\sum_{k=1}^{\left\lfloor \frac{n-1}{2} \right\rfloor} 2[4(2n-(2k-1))]\right] + 4(n+1) & for\ n \geq 4. \end{cases}$$

Proof. We can calculate the eccentricity connectivity index of $G = L(L_n)$ using Table [1-3] respectively. This criterion is similar to that of Theorem 2.1. Using $\deg(u)$ instead of $\deg^{De}(u)$ to obtain the desired result. The following graphical layout shows the comparison between distance eccentricity connectivity index and eccentricity connectivity index of $L(L_n)$.

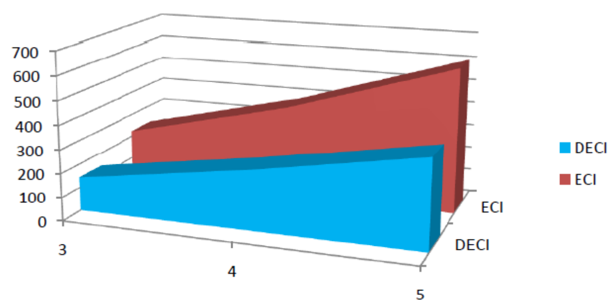

Figure 2. Graphical representation of DECI and ECI of linear chain of n benzene $L(L_n)$.

Lemma 2.3. *For* $n \geq 3$ *in the graph* $G = L(L_n)$, *the relation between* $\xi^C(G)$ *and* $\xi^{De}(G)$ *is given by* $\xi^C(G) > \xi^{De}(G)$.

Lemma 2.4. *Let* $G = L(L_n)$, $n \geq 3$. *Then*

$$\xi^{De}(G) = \begin{cases} \sum_{k=1}^{n} 4[(2n-(k-1))^2] + \sum_{k=1}^{\left\lfloor \frac{n}{2} \right\rfloor + 1} 2[(n+2k)] & \textit{for } n \geq 3 \\ \sum_{k=1}^{n} 4[(2n-(k-1))^2] + \left[\sum_{k=1}^{\frac{n}{2}} 2(n+(2k-2))^2 \right] + (n+1)^2 & \textit{for } n \geq 4. \end{cases}$$

Proof. Using the definition of $\xi_1(G)$ and Table [1-3], we obtained the exact result.

Lemma 2.5. *Let* $G = (L(L_n)),\ n \geq 3$. *Then*

$$\deg^{De}(u) = \begin{cases} 2,\ u \in V_e^{2n-(k-1)},\ 1 \leq k \leq n, & \textit{for all } n \\ 1,\ u \in V_e^{n+2k},\ 1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor + 1, & \textit{for odd } n \\ 1,\ u \in V_e^{n+2k-1},\ 1 \leq k \leq \frac{n}{2}, & \textit{for even } n \\ 2,\ u \in V_e^{n+1}, & \textit{for even } n \end{cases}$$

Proof. Clearly V_e^{α} is a set of nodes whose eccentricity is equal to α. For all n, when $e(u) = 2n-(k-1),\ 1 \leq k \leq n$ then $\deg^{De}(u) = 2$; For odd n, when $e(u) = n+2k,\ 1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor + 1$ then $\deg^{De}(u) = 1$. Also, for even n when $e(u) = n+2k-1,\ 1 \leq k \leq \frac{n}{2}$ then $\deg^{De}(u) = 1$; again for even n, when $e(u) = n+1$ then $\deg^{De}(u) = 2$.

Lemma 2.6. *Let* $G = (L(L_n)),\ n \geq 3$. *Then* $Q(G) = \begin{cases} 9n+1 & \textit{for } n \geq 3 \\ 9n+2 & \textit{for } n \geq 4. \end{cases}$

Proof. As we previously discussed in Theorem 2.1, for odd n, there are n sets consists of four vertices each have $\deg^{De}(u) = 2$ and $\left(\frac{n+1}{2}\right)$ sets consists of two vertices each have $\deg^{De}(u) = 1$. Now, $Q(G) = \sum_{u \in V(G)} \deg^{De}(u)$ $= 4n(2) + 2\left(\frac{n+1}{2}\right)(1) = 9n+1$. For even n, there are n sets consists of four vertices each have $\deg^{De}(u) = 2$ and $\left(\frac{n}{2}\right)$ sets consists of two vertices each have $\deg^{De}(u) = 1$. Also in the second row of $L(L_n)$, central vertex have $\deg^{De}(u) = 2$. Therefore, $Q(G) = \sum_{u \in V(G)} \deg^{De}(u) = 4n(2) + 2\left(\frac{n}{2}\right)(1) + 2 = 9n + 2$.

Remark (1). Let $G = (L(L_n))$, $n \geq 3$ be a line graph of L_n with $\delta^{De}(G) = 1 < \deg^{De}(u) < 2 = \Delta^{De}(G)$ and $\delta(G) = 2 < \deg(u) < 4 = \Delta(G)$. Then $\sum_{u \in V(G)} \deg^{De}(u) < \sum_{u \in V(G)} \deg(u)$.

Lemma 2.7. *Let* $G = (L(L_n))$, $n \geq 3$. *Then* $M_1^{De}(G)$

$$= \begin{cases} 17n + 1 & \textit{for } n \geq 3 \\ 17n + 4 & \textit{for } n \geq 4. \end{cases}$$

Remark (2). Let $G = (L(L_n))$, $n \geq 3$. Then $M_1^{De}(G) > Q(G)$.

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