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The Eccentric Connectivity and Balaban Indices of an Infinite Family of Nanotorus

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ABSTRACT

Let $G=(V,E)$ be a graph, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges. For $u \in V(G)$, defined $d(u)$ be degree of vertex u. The eccentricity connectivity index of a molecular graph G is defined as $\xi^c(G) = \sum_{u \in V(G)} \deg_G(u) \cdot ecc(u)$, where $ecc(u)$ is defined as the length of u maximal path connecting a to another vertex of G. The Balaban index of a graph G is defined as $J(G)= \frac{m}{\mu+1}\sum_{e=uv}[d(u)d(v)]^{-0.5}$, where m is the number of edges of G, μ is the cyclomatic number of G and for every vertex x of G, $d(x)$ is the summation of distances between x and all vertices of G. In this paper, we computing eccentricity connectivity and balaban indices for linear polycene parallelogram graph of benzenoid by a new method.

KEYWORDS: Eccentricity connectivity, Balaban index, Polycene parallelogram

1 INTRODUCTION

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. The vertices in G are connected by an edge if there exists an edge $uv \in E(G)$ connecting the vertices u and v in G such that $u,v \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by $|V(G)|$ and $|E(G)|$, respectively.

A topological index is a real number related to a molecular graph, which is a graph invariant. There are several topological indices already defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of the molecules. The Wiener index is the first topological index proposed to be used in Chemistry. It was introduced in 1947 by Harold Wiener, as the path number for characterization of alkenes. It is defined as the sum of distances between all pairs of vertices in the graph under consideration. In the 1990s, a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to W. The eccentric connectivity index of the molecular graph *G*, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [9]. It is defined as $\xi^c(G)=\sum_{u\in V(G)}\deg_G(u).ecc(u)$ where $deg_G(u)$ denotes the degree of the vertex *u* in *G* and *ecc(u)*= *Max{d(x,u) | x* $\in$ *V(G)}*. The radius and diameter of *G* are defined as the minimum and maximum eccentricity among vertices of *G*, respectively [6-12]. Define the eccentric connectivity polynomial of a graph *G*, *ECP(G,x)*, as *ECP(G,x)*= $\sum_{u\in V(G)}\deg_G(u)x^{ecc(u)}$. Then the eccentric connectivity index is the first derivative of *ECP(G,x)* evaluated at *x = 1*. The Balaban index [1–5] of a graph G is defined as $J(G)=\frac{m}{\mu+1}\sum_{e=uv}[d(u)d(v)]^{-0.5}$ where *m* is the number of edges of *G* and μ *(G)* = *E(G)−V(G)+1* is the cyclomatic number of *G*.

2 MAIN RESULTS

In this section is to compute $\xi^c(G)$, and *J(G)* for an infinite family of linear polycene parallalogram of benzenoid graph [2]. To do this we should to consider the following examples:

Example 1. Consider linear polycene parallelogram benzenoid graph $L_2[G]$ depicted in Fig. 1. This graph has *16* vertices and *19* edges. This graph has two vertices with eccentricity *4* and degree *3*, two vertices with eccentricity *7* and degree *2*, *8* vertices with eccentricity *5* such that four vertices with degree *2* and four vertices with degree *3*. And four vertices of eccentricity *6* and degree *2*. Then

$$ECP(L_2[G],x)=6x^4+20x^5+8x^6+4x^7 \quad \text{and} \quad \xi^c(L_2[G]) = ECP(L_2[G],1)=200$$

Also this graph contain three case of edges e_1, e_2 and e_3, such that d(u)=d(v)=2, d(u)=d(v)=3 and d(u)=2, d(v)=3 respectively for uv from e_1, e_2 , e_3 and $|e_1|=6$, $|e_2|=5$ and $|e_3|=8$ then

$$J(L_2[G])=19/4[6(2.2)^{-0.5}+8(2.3)^{-0.5}+5(3.3)^{-0.5}]=\frac{19}{4}\left(3+\frac{5}{3}+\frac{8}{\sqrt{6}}\right)$$

Example 2. Consider linear polycene parallelogram benzenoid graph $L_3[G]$ depicted in Fig. 2. This graph has *30* vertices and *38* edges. Cardinal $|e_1|=6$, $|e_2|=16$ and $|e_3|=16$ then by computing eccentricity of $L_3[G]$ it is easy to check that

$$ECP(L_3[G],x)=4x^{11}+8x^{10}+12x^9+14x^8+26x^7+12x^6 \quad \text{and} \quad \xi^c(L_3[G]) = ECP'(L_3[G],1)=598$$

and by computing balaban index we have

$$J(L_3[G])=38/9[6(2.2)^{-0.5}+16(2.3)^{0-/5}+16(3.3)^{-0.5}]=\frac{38}{9}\left(3+\frac{16}{3}+\frac{16}{\sqrt{6}}\right).$$

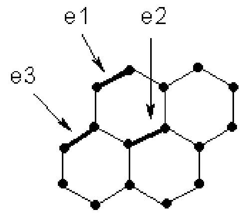

Fig.1

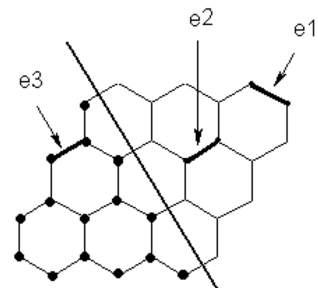

Fig.2

Example 3. Consider linear polycene parallelogram benzenoid graph $L_4[G]$ depicted in Fig.3. This graph has 48 vertices and 63 edges and *Max ecc(u)=15* , *Min ecc(u)= 8*. Also Cardinal $|e_1|=6$, $|e_2|=4\times 6=24$ and $|e_3|=(4\times 3)+(3\times 7)=33$. Then $ECP(L_4[G],x)=4x^{15}+8x^{14}+12x^{13}+14x^{12}+18x^{11}+20x^{10}+32x^{9}+18x^{8}$. So $\xi^c(L_4[G])$ =ECP'(L_4[G],1)=1326
and by computing balaban index we have

$$J(L_4[G])=63/16[6(2.2)^{-0.5}+24(2.3)^{-0.5}+33(3.3)^{-0.5}]=\frac{63}{16}\left(3+\frac{33}{3}+\frac{24}{\sqrt{6}}\right)$$

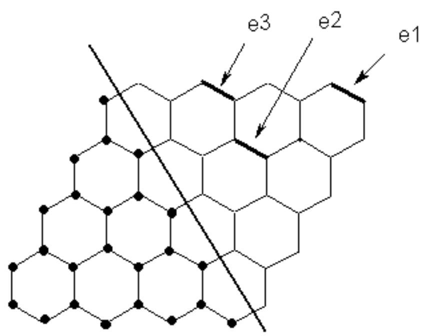

Fig.3

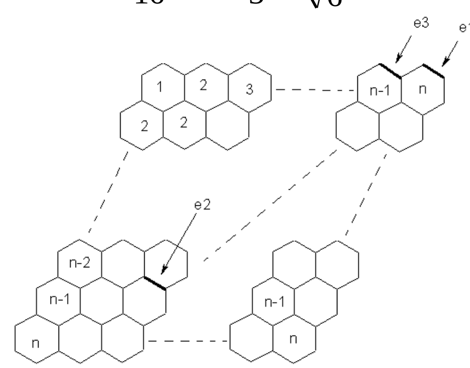

Fig.4. 2-Dimensional Graph of Polycene Parallelogram nanotorus

In generally consider linear polycene parallelogram benzenoid graph $L_n[G]$ depicted in Fig.4. This graph has $|V|=2n(n+2)$ and $|E|=3n^2+4n-1$. For computing the eccentric connectivity index and balaban index for $L_n[G]$ in total case, we using a new method.
In this method we compute maximum, minimum eccentric connectivity and cardinal three case of edges e_1, e_2 and e_3 for linear polycene parallelogram benzenoid graph $L_n[G]$. We have for $u\in V(L_n[G])$, *Max ecc(u)=4n-1* and *Min ecc(u)= 2n*.

In Fig.5, one can see the eccentric connectivity index for every $u\in V(L_n[G])$ and in Fig.4, one can see several deictic line for computing the eccentric connectivity index. First line starting of Max *ecc(u)=4n-2* and finally with *ecc(u)=2n+1*. and for secondly line, starting of *ecc(u)=4n-2* and finally with *ecc(u)=2n*. Similarly for another lines we can computing eccentric connectivity index. For vertices, with eccentric connectivity index *4n-1, 4n-2, 4n-4, 4n-6,…, 2n+2, 2n+1*, we have *deg(u)= 2* and for another vertices we have *deg(u)=3*, where $u\in V(L_n(G))$. Then by using of Fig.4,5, we have table (1) for eccentric connectivity index of graph.

Tabel (1): *Eccentric connectivity index for vertices $L_n[G]$*

<u>*4n-1*</u>	<u>*4n-2*</u>	*4n-3*	*4n-4*	*4n-5*	*4n-6*	...	*2n+2*	*2n+1*	<u>*2n+1*</u>
	<u>*4n-2*</u>	*4n-3*	*4n-4*	*4n-5*	*4n-6*	...	*2n+2*	*2n+1*	*2n*
			<u>*4n-4*</u>	*4n-5*	*4n-6*	...	*2n+2*	*2n+1*	*2n*
				4n-5	*4n-6*	...	*2n+2*	*2n+1*	*2n*
							.	.	.
							.	.	.
							.	.	.
							<u>*2n+2*</u>	*2n+1*	*2n*
								<u>*2n+1*</u>	

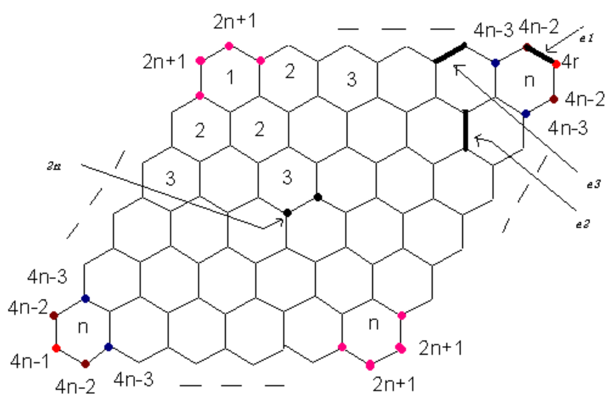

Fig.5

By using in this method one can see the eccentricity connectivity index for an infinite family of linear polycene parallelogram benzenoid graph is as follows:

$$\xi^c(L_n[G]) = 2[(4n-1)+2(4n-2)+(4n-3)+(4n-6)+\ldots+(2n+3)+(2n+2)+2(2n+1)]$$
$$+6[(n-1)2n+n(2n+1)+5(n-1)+9(n-2)+13(n-3)+\ldots+3(4n-11)+2(4n-7)].$$

By arrangement above formula, we have:

$$\xi^c(L_n[G]) = \sum_{k=0}^{n-2} 24(n^2-k^2) + \sum_{k=0}^{n-2}(n-k) + \sum_{k=0}^{2n-2} 4(2n+k) + 20n - 12$$

Thus

$$\xi^c(L_n[G]) = 24n^3 - 31n^2 + 18n - 28 - \sum_{k=0}^{n-2}(24k^2+k) + \sum_{k=0}^{2n-2} 4k$$

Now we computing balaban index for this molecular graph**.** With respect Fig.4, we have $2n(n+2)$ vertices and $3n^2+4n-1$ edges. Also this graph has only three case of edge and cardinal for every $e=uv \in E$ equal $|e_1|=6$, $|e_2|=4(2(n-1))=8(n-1)$ and $|e_3|=(2n-1)(n-1)+n(n-1)=(3n-1)(n-1)$. Thus $m=3n^2+4n-1$ and $\mu=(3n^2+4n+1)-2n(n+2)+1=n^2+1$. So we have:

$$J(L_n[G])=\frac{3n^2+4n-1}{n^2+1}\left(6\times(2\times2)^{-0.5}+8(n-1)\times(3\times3)^{-0.5}+(3n-1)\times(n-1)\times(3\times2)^{-0.5}\right)$$

$$J(L_n[G])=\frac{3n^2+4n-1}{n^2+1}\left(\frac{8n+1}{3}+\frac{(3n-1)(n-1)}{\sqrt{6}}\right)$$

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