Computing modified eccentric connectivity polynomial of one-square carbon nanocones by use a numerical method

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The Modified Eccentric Connectivity Polynomial of a molecular graph, G, is defined as *MECP(G,x)*= $\sum_{u \in V(G)}$ $n_G(u)$. $x^{ecc(u)}$, where *ecc(u)* is defined as the length of a maximal path connecting *u* to another vertex of molecular graph *G* and $n_G(u)$ is the sum of the degrees of its neighborhoods. Suppose CNC4[n] is carbon nanocone with a unique square. In this paper, we compute this polynomial for $CNC_4[n]$ carbon nanocones.

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1. Introduction

Research into carbon nanocones (CNC) started almost at the same time as the discovery of carbon nanotube (CNT) in 1991. Ball studied the closure of CNT and mentioned that CNT could sealed by a conical cap, see [1]. The official report of the discovery of isolated CNC was made in 1994, when Ge and Sattler from the University of Hawaii reported their observations of carbon cones mixed together with tubules on a flat graphite surface, see [12].

The heights of the cones exceeded those of any other carbon cones in the literature, and the apex angles of the CNC were widely distributed. These findings supported the explanation of the opening angles of the five angles having cone-helix structures.

The closure of the tip requires the inclusion of a pentagon, which is converted from a hexagon to create a cone with an opening angel of 112.9°. This process can be continued by introducing more pentagons into the graphitic sheet with corresponding 60° disclamations for each additional pentagon up to a total of five pentagons. If a 120° wedge is considered then a cone with a single square defect at the apex is obtained, [18,19,20,22,24,25]. See Fig. 1 [23].

A topological index of a molecular graph *G* is a numeric quantity related to *G*. The oldest nontrivial topological index is the Wiener index which was introduced by Harold Wiener [15,16]. John Platt was the only person who immediately realized the importance of the Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the Wiener index. The name of topological index was introduced by Hosoya [14,20].

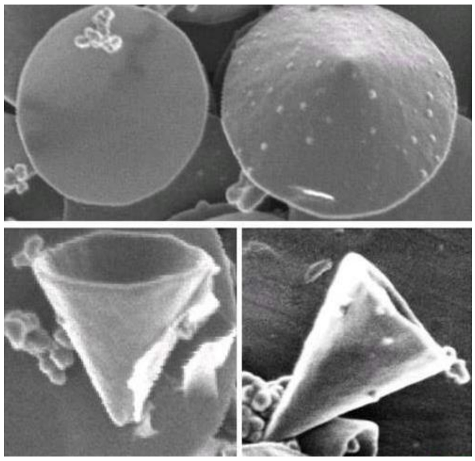

Fig. 1.

Many topological indices have been defined and several applications of them have been found in physical, chemical and pharmaceutical models and other properties of molecules.

The eccentric connectivity index of the molecular graph *G*, $\xi^c(G)$, was proposed by Sharma, Goswami and Madan [16]. 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.

The modified eccentric connectivity polynomial (MECP) of graph G is defined as MECP(G,x)=$\sum_{u \in V(G)} n_G(u) x^{ecc(u)}$, where $n_G(u)$ is the sum of the degrees of its neighborhoods [2].

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by $V(G)$ and $E(G)$, respectively. 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 so 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 defined by $|V(G)|$ and $|E(G)|$ respectively. In graph theory, a path of length n in a graph is a sequence of $n + 1$ vertices such that from each of its vertices there is an edge to the next vertex in the sequence. For two vertices u and v of G, $d_G(u,v)$ denotes the length of a minimal path connecting u and v. A graph G is called connected, if there is a path connecting vertices u and v of G, for every $u,v \in V(G)$. Suppose H is a set, H_i, $1 \leq i \leq m$, are subsets of H and $K=\{H_i\}_{1\leq i\leq m}$ is a family of subsets of H. If H_i's are non-empty, $H=\bigcup_{i=1}^{m} H_i$ and $H_i \bigcap H_j = \Phi$ *(empty)*, for $i \neq j$ then K is called a partition of H, [17,4].

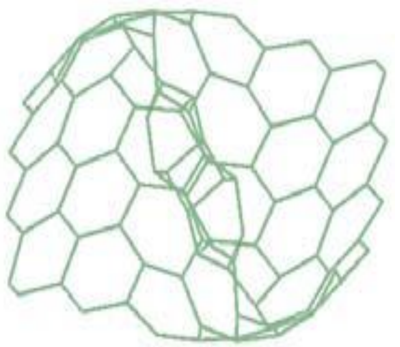

Fig. 2. The carbon nanocone $CNC_4[4]$.

2. Main results and discussion

In this section we calculate the MEC polynomials of One–Square,Carbon Nanocone by use a numerical method. In continue a matlab program is presented which is useful for computing the MEC polynomial of a nanocone. We apply this program to compute of the molecular graph of nanocone $CNC_4[n]$, when $1 \leq n$, see Fig. 2.

Lemma 1. For $u \in V(CNC_4[n])$**,**

Max ecc(u)=4n-2 and Min ecc(u)= 2n.

Proof. Suppose u is a vertex of the central of $CNC_4[n]$. Then from Fig. 2, one can see that there exists a vertex v of degree 2 such that d(u,v)=2n and there exists another vertex w of degree 2 such that d(u,w) =2n-2. Therefore, the shortest path with maximum length is connecting two vertices of degree 2 in $CNC_4[n]$. Then this proof is complete.

Theorem 1. The MEC polynomial of one–square carbon nanocone is computed as follows:

$MECP(CNC_4[n],x)=$

$$\frac{4(6n-2)x^{4n}}{x^2}+\frac{4(n-1)(7x+9)x^{4n}}{x^4}+\frac{36(1+x)x^{4n}}{x^2}\times\sum_{i=2}^{n-1}\frac{n-i}{x^{2i}}$$

Proof. Suppose $K[n]= CNC_4[n]$. With respect to Fig. 3, $K[n]=\bigcup_{i=1}^{4} T_i$, where $\{T_i\}_{1\leq i\leq 4}$ is a partition of the molecular graph K[n]. We have $|V(K[n])|=4n^2$ and $|E(K[n])|=2(3n^2-n)$. It is easy to check that, deg(u)=2 for vertices with maximum eccentric connectivity and deg(u)=3 for other vertices of T_i. See Table 1 for vertices of T_i.

Table 1. Types of $CNC_4[n]$ vertices.

Vertex	Number	Ecc	Degree
Type 1	4n	4n-2	2
Type i+1,A $1\leq i\leq n-1$	4n-4i	4n-2i-1	3
Type i+1 ,B $1\leq i\leq n-1$	4n-4i	4n-2i-2	3

Thus implies that

$$MECP(T_i,x)=\sum_{u\in V(T_i)} n_G(u)x^{ecc(u)}$$

$$=(6n-2)x^{4n-2}+7(n-1)x^{4n-3}+9(n-1)x^{4n-4}+9(n-2)x^{4n-5}+9(n-2)x^{4n-6}+\ldots+9\times 2x^{2n+3}+9\times 2x^{2n+2}+9x^{2n+1}+9x^{2n}$$

$$=(6n-2)x^{4n-2}+(n-1)(7x+9)x^{4n-4}+9(n-2)(1+x)x^{4n-6}+\ldots+9\times 2(1+x)x^{2n+2}+9(1+x)x^{2n}$$

$$=(6n-2)x^{4n-2}+(n-1)(7x+9)x^{4n-4}+9(1+x)x^{4n-2}\sum_{i=2}^{n-1}\frac{n-i}{x^{2i}}$$

Therefore

$$MECP(K[n],x)=\sum_{u\in V(K[n])} n_G(u)x^{ecc(u)}$$

$$=4\times MECP(T_i,x)=4\times\sum_{u\in V(T_i)} n_G(u)x^{ecc(u)}$$

$$=4(6n-2)x^{4n-2}+4(n-1)(7x+9)x^{4n-4}+36(1+x)x^{4n-2}\sum_{i=2}^{n-1}\frac{n-i}{x^{2i}}$$

Then this proof is completed.

In this section we determine a matlab Program for computing the modified eccentric connectivity polynomial of $CNC_4[n]$ carbon nanocones.

function [varargout]=MEC Polynomial (varargin)

```
 %      cnc4(1:10,'plot',...
 %     'LimitN',[1 3 4 5],...
 %     'Axis',[x_min x_max y_min y_max],...
 %      'Grid')
 nn = varargin{1};
syms x
if ischar(varargin{1}) == 1
 error('Error : Vector must have 1 Argument.')
else
nn = varargin{1};
nn2 = nn;
end
F_P = strcmp(varargin,'Limit') ;
if sum(F_P) ~=0 ; nn2 = varargin{find(F_P)+1} ;
endif size(nn,1) ~= 1
error('Error : Vector(N) must have 1 row.')
elseif ( min(nn) < 1 )
error('Error : N >=1 ')
elseif (min(nn2) < min(nn)) || (max(nn2) > max(nn))
error('Error : N2 ')
else
%%%  Modified Eccentlic Connectivity Polynomial
 for j = 1:length(nn)
 n=nn(j);
Sigma = sum([0 ((n-(2:n-1))./(x.^(2.*(2:n-1))))]);
ANS.MECPx(n-nn(1)+1) =
(((4*((6*n)-2)*(x^(4*n)))/(x^2))+((4*(n-
1)*((7*x)+9)*(x^(4*n)))/(x^4))+((36*(1+x)*(x^(4*n)))/(x^
2))*Sigma;
end
if nargout <= 1
varargout{1}.MECPx          =          ANS.MECPx          ;
ANS.MECPxNAME = '.MECPx';
else
varargout{1}  =  ANS.MECPx  ;  ANS.MECPxNAME  =
'ARG1'; end.
```

In Table 2 we calculate the MEC polynomials of $CNC_4[n]$ for $1 \le n \le 10$, and Fig. 3, the diagram of the MEC polynomials of $CNC_4[n]$ are depicted.

Table 2. The MEC Polynomial of $CNC_4[n]$.

n	MEC Polynomial
1	$16x^{2}$
2	$40x^{6}+28x^{5}+36x^{4}$
3	$64x^{10}+56x^{9}+72x^{8}+36x^{7}+36x^{6}$
4	$88x^{14}+84x^{13}+108x^{12}+72x^{11}+72x^{10}+36x^{9}+36x^{8}$
5	$108x^{18}+102x^{17}+144x^{16}+108x^{15}+108x^{14}+72x^{13}+72x^{12}+36x^{11}+36x^{10}$
6	$136x^{22}+140x^{21}+180x^{20}+144x^{19}+144x^{18}+108x^{17}+108x^{16}+72x^{15}+72x^{14}+36x^{13}+36x^{12}$
7	$160x^{26}+168x^{25}+216x^{24}+180x^{23}+180x^{22}+144x^{21}+144x^{20}+108x^{19}+108x^{18}+72x^{17}+72x^{16}+36x^{15}+36x^{14}$
8	$184x^{30}+196x^{29}+252x^{28}+216x^{27}+216x^{26}+180x^{25}+180x^{24}+144x^{23}+144x^{22}+108x^{21}+108x^{20}+72x^{19}+72x^{18}+36x^{17}+36x^{16}$
9	$208x^{34}+224x^{33}+288x^{32}+252x^{31}+252x^{30}+216x^{29}+216x^{28}+180x^{27}+180x^{26}+144x^{25}+144x^{24}+108x^{23}+108x^{22}+72x^{21}+72x^{20}+36x^{19}+36x^{18}$
10	$232x^{38}+252x^{37}+324x^{36}+288x^{35}+288x^{34}+252x^{331}+252x^{32}+216x^{31}+216x^{30}+180x^{29}+180x^{28}+144x^{27}+144x^{26}+108x^{25}+108x^{24}+72x^{23}+72x^{22}+36x^{21}+36x^{20}$

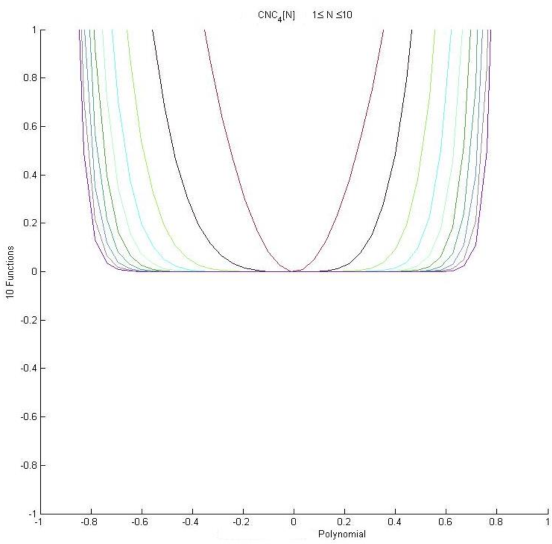

Fig. 3. The diagram of the MEC polynomial of $CNC_4[n]$ for $1 \le n \le 10$.

3. Conclusions

In this paper, we calculated the MEC polynomials of one–square carbon nanocone by use a Matlab program. Our numerical method is general and can be extended to other nano-materials too. On the other hand, by using this matlab program, can be calculated modified eccentric connectivity polynomial for carbon nanocone of any arbitrary capacities.

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