

RESEARCH ARTICLE

Computational aspects of line graph of carbon nanocones

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Submitted: 24 March 2017; Revised: 23 September 2018; Accepted: 23 August 2019

Abstract: Graph theory plays substantial role in mathematics, chemistry, QSAR and physical sciences. The basic layout of the graph theoretic model is a molecular structure in which vertices of the graph correspond to atoms, and edges correspond to chemical bonds. The study of this graph model provides information about the chemical structure. A line graph has many useful applications in physical chemistry. M-polynomial is rich in producing closed forms of many degree-based topological indices which correlates chemical properties of the material under investigation. This polynomial is used in computing closed formulas of many degree-based topological invariants of the molecular structures. The molecular graph of carbon nanocones has a conical structure with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its centre. In this study, we transformed the molecular structure of carbon nanocones into graph theoretic model and produced its line graph. Thereafter, we determined closed formulas for M-polynomials of line graphs of nanocones. We also recovered important topological degree-based indices of the line graph of nanocones. Moreover, we provide different graphs of topological indices and their relations with the parameters of the line graph of nanocones. These graphs depict the actual dependencies of the topological indices on the parameters of the carbon nanocones.

Keywords: Degree-based topological index, general Randic index, line graph, M-polynomial, symmetric division index, Zagreb index.

INTRODUCTION

In mathematical chemistry, mathematical tools such as polynomials and numbers predict properties of compounds without using quantum mechanics. These tools, in combination, capture information hidden in the symmetry of molecular graphs. Topological indices are numerical parameters of a graph, which characterise its topology and are usually graph invariant. They describe the structure of molecules numerically and are used in the development of qualitative structure activity relationships (QSARs). The most commonly known invariants of such kind are degree-based topological indices. These are actually the numerical values that correlate the structure with various physical properties, chemical reactivity, and biological activities (Klavžar & Gutman, 1996; Rucker & Rucker, 1999; Brückler *et al.*, 2011). It is an established fact that many properties such as heat of formation, boiling point, strain energy, rigidity and fracture toughness of a molecule are strongly connected to its graphical structure and this fact plays a synergic role in chemical graph theory.

Several algebraic polynomials have useful applications in chemistry such as Hosoya polynomial (also called Wiener polynomial) (Gutman, 1993),

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which play a vital role in determining distance-based topological indices. Among other algebraic polynomials, M-polynomial (Deutsch & Klavzar, 2015) introduced in 2015, plays the same role in determining the closed form of many degree-based topological indices (Munir et al. 2016a, b, c, d, 2017; Kwun et al., 2017; Ali et al., 2018). The main advantage of M-polynomial is the wealth of information that it contains about degree-based graph invariants.

Carbon nanocones have been observed since 1968 or even earlier (Gillot et al., 1968) on the surface of naturally occurring graphite. Their bases are attached to the graphite and the height varies between 1 to 40 micrometers. The walls are often curved and are less regular than those of the laboratory made nanocones. Carbon nanostructures have attracted considerable attention due to their potential uses in many applications including energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes (Iijima, 1991). Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices (Zhao et al., 2002; Adisa et al., 2011). More recently, carbon nanocones have gained increased scientific interests due to their unique properties and promising uses in many novel applications such as energy and gas storage. Figure 1 depicts the structure of a carbon nanocone.

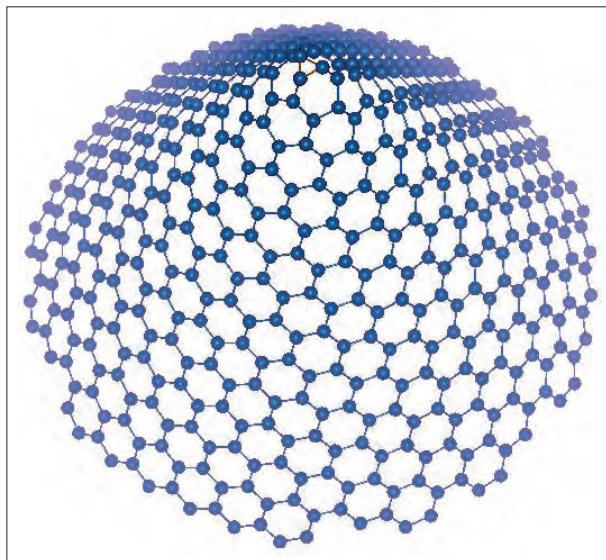


Figure 1: Carbon nanocone $CNC_k[n]$

The molecular graph of $CNC_k[n]$ nanocones has a conical structure with a cycle of length k at its core and n layers of hexagons placed at the conical surface around its centre as shown in Figure 2.

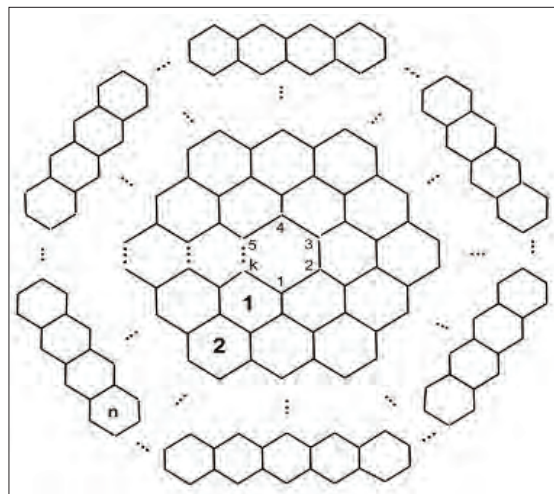


Figure 2: Carbon nanocones $CNC_k[n]$

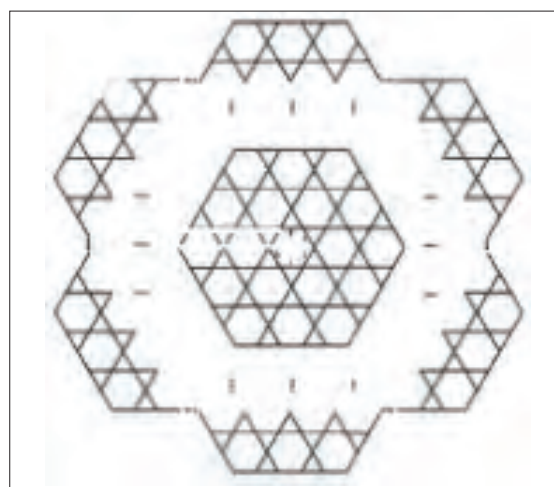


Figure 3: Line graph of the carbon nanocones $CNC_k[n]$

The line graph $L(G)$ of a graph G is the graph each of whose vertices represents an edge of G and two of its vertices are adjacent if their corresponding edges are adjacent in G (Iranmanesh et al., 2009; Huo et al., 2016). In Figure 3, we can see the line graph of the carbon nanocones $CNC_k[n]$.

The present paper is concerned with the line graph of the carbon nanocone $CNC_k[n]$ where k is the number of hexagons forming the base of the cone and n is the number of layers of the cone. In Wu *et al.* (2010), authors computed the Wiener index of a graph defined as $W(G) = \sum_{\{u,v\} \subset V(G)} d_G(u,v)$. They also computed the Wiener index of the line graph and established new bounds on the Wiener index of the line graph of any graph. In Buckley and Rapoport (1981), authors computed mean distances in line graphs. In Cataldo *et al.* (2010), Wiener index was used as pure topological potential energy of graphenic infinite structures producing interesting results, assigning to fullerene-like nanostructures a non-negligible probability of formation on graphene sheets on carbon black or on amorphous carbon in general. Authors also showed that 1-pentagonal nanocones become chemically reactive when it reaches certain sizes. Ashrafi and Mohammad-Abadi (2012) computed Wiener index of 1-pentagonal nanocones.

In this paper, we compute M-polynomial and degree-based topological indices of the line graph of nanocones. We also give many degree-based topological indices in closed forms for the line graphs of nanocones.

METHODOLOGY, RESULTS AND DISCUSSION

Throughout this paper, G is a connected graph, $V(G)$ and $E(G)$ are the vertex set and edge set, respectively and d_v denotes the degree of a vertex v .

Definition 1. (Deutsch & Klavzar, 2015). The M-polynomial of G is defined as:

$$M(G, x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G) x^i y^j$$

where $\delta = \text{Min}\{d_v \mid v \in V(G)\}$, $\Delta = \text{Max}\{d_v \mid v \in V(G)\}$, and $m_{ij}(G)$ is the edge $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$.

The first topological index was introduced by Wiener (1947) and it was named *path number*, which is now known as *Wiener index*. In chemical graph theory, this is the most studied molecular topological index due to its wide applications [see for details (Gutman & Polansky, 1986; Dobrynin *et al.*, 2001)]. Randić index, (Randić, 1975) denoted by $R_{-1/2}(G)$ and introduced by Milan Randić in 1975 is also one of the oldest topological indices. The Randić index is defined as:

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

Working independently, Bollobas and Erdos (1998) and Amić *et al.* (1998) proposed the generalised Randić index and it has been studied extensively by both chemists and mathematicians (Hu *et al.*, 2005). Many mathematical properties have been discussed (Caporossi *et al.*, 2003). For a detailed survey, we refer the book (Li *et al.*, 2006).

The general Randić index is defined as:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha, \text{ and the inverse Randić index is defined as } RR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}. \text{ Here } \alpha \text{ can be any real number. Obviously } R_{-1/2}(G) \text{ is the particular case of } R_\alpha(G) \text{ when } \alpha = -\frac{1}{2}.$$

The Randić index is the most popular, most often applied and most studied among all other topological indices. Many papers and books such as Kier and Hall (1976;1986) are written on this topological index. Randić himself wrote two reviews on his Randić index (Randić, 2001; 2008) and there are more reviews (for example Li & Shi, 2008). The suitability of the Randić index for drug design was immediately recognised, and eventually, the index was used for this purpose on countless occasions. The physical reason for the success of such a simple graph invariant is still an enigma, although several more-or-less plausible explanations were offered.

Gutman and Trinajstić (1972) introduced the first Zagreb index and second Zagreb index, which are defined as: $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$ and

$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$, respectively. The second modified Zagreb index is defined as:

$${}^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$$

For details about these indices, we refer Nikolić *et al.*, (2003), Gutman and Das (2004) and Zhou and Trinajstić (2010) to the readers.

The symmetric division index is defined as:

$$SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)} \right\}$$

Another variant of Randic index is the harmonic index defined as:

$$H(G) = \sum_{vu \in E(G)} \frac{2}{d_u + d_v}.$$

The Inverse sum-index is defined as:

$$I(G) = \sum_{vu \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

The augmented Zagreb index is defined as:

$$A(G) = \sum_{vu \in E(G)} \left\{ \frac{d_u d_v}{d_u + d_v - 2} \right\}^3,$$

and it is useful for computing heat of formation of alkanes. [For details about these topological indices we refer (Rehman et al., 2017; Sardar et al., 2017; De, 2018)].

Table 1 relates some well-known degree-based topological indices with M-polynomial (Deutsch & Klavzar, 2015).

where

$$D_x = x \frac{\partial(f(x, y))}{\partial x},$$

$$D_y = y \frac{\partial(f(x, y))}{\partial y},$$

$$S_x = \int_0^x \frac{f(t, y)}{t} dt,$$

$$S_y = \int_0^y \frac{f(x, t)}{t} dt,$$

$$J(f(x, y)) = f(x, x),$$

$$Q_\alpha(f(x, y)) = x^\alpha f(x, y).$$

A graph uses points connected by lines to show how something changes in value (as time goes by, or as something else happens). Line graph of the carbon nanocone is shown in figure 3. Let $G = L(CNC_k[n])$ be the line graph of carbon nanocones $CNC_k[n]$. From Figure 3, we see that the graph has $8k+2kn$ number of vertices and $k(n+1)(3n+1)$ number of edges. The vertex partition and edge partition of graph G are shown in Tables 1 and 2, respectively.

Let $G = L(CNC_k[n])$ be the line graph of the carbon nanocones $CNC_k[n]$. Then the M-polynomial of

$L(CNC_k[n])$ is,

$$M(L(CNC_k[n]); x, y) = 2kx^2y^3 + k(2n-1)x^3y^3 + 2knx^3y^4 + 3kn^2x^4y^4.$$

Proof

Let $L(CNC_k[n])$ be the line graph of the carbon nanocones $CNC_k[n]$. It is easy to see from Figure 3 that,

$$|V(L(CNC_k[n]))| = 8k + 2kn$$

$$|E(L(CNC_k[n]))| = k(n+1)(3n+1)$$

From Table 2, the vertex set of $L(CNC_k[n])$ have three partitions:

$$V_1(L(CNC_k[n])) = \{u \in V(L(CNC_k[n])) : d_u = 2\},$$

$$V_2(L(CNC_k[n])) = \{u \in V(L(CNC_k[n])) : d_u = 3\},$$

$$V_3(L(CNC_k[n])) = \{u \in V(L(CNC_k[n])) : d_u = 4\},$$

such that,

$$|V_1(L(CNC_k[n]))| = k,$$

$$|V_2(L(CNC_k[n]))| = 2kn,$$

$$|V_3(L(CNC_k[n]))| = 7k.$$

From Table 3, the edge set of $L(CNC_k[n])$ have four partitions:

$$E_1(L(CNC_k[n])) = \{e = uv \in E(L(CNC_k[n])) : d_u = 2, d_v = 3\},$$

$$E_2(L(CNC_k[n])) = \{e = uv \in E(L(CNC_k[n])) : d_u = d_v = 3\},$$

$$E_3(L(CNC_k[n])) = \{e = uv \in E(L(CNC_k[n])) : d_u = 3, d_v = 4\},$$

$$E_4(L(CNC_k[n])) = \{e = uv \in E(L(CNC_k[n])) : d_u = d_v = 4\},$$

such that,

$$|E_1(L(CNC_k[n]))| = 2k,$$

$$|E_2(L(CNC_k[n]))| = k(2n-1),$$

$$|E_3(L(CNC_k[n]))| = 2kn,$$

$$|E_4(L(CNC_k[n]))| = 3kn^2,$$

Table 1: Derivation of some degree-based topological indices from M-polynomial

Topological index	Derivation from $M(G; x, y)$
First Zagreb	$(D_x + D_y)(M(G; x, y))_{x=y=1}$
Second Zagreb	$(D_x D_y)(M(G; x, y))_{x=y=1}$
Second modified Zagreb	$(S_x S_y)(M(G; x, y))_{x=y=1}$
Inverse Randic $\alpha \in \mathbb{N}$	$(D_x^\alpha D_y^\alpha)(M(G; x, y))_{x=y=1}$
General Randic $\dot{c} \alpha \in \mathbb{N} \alpha \in \mathbb{N}$	$(S_x^\alpha S_y^\alpha)(M(G; x, y))_{x=y=1}$
Symmetric division index	$(D_x S_y + S_x D_y)(M(G; x, y))_{x=y=1}$
Harmonic index	$2S_x J(M(G; x, y))_{x=1}$
Inverse sum index	$S_x J D_x D_y(M(G; x, y))_{x=1}$
Augmented Zagreb index	$S_x^3 Q_{-2} J D_x^3 D_y^3(M(G; x, y))_{x=1}$

Table 2: The partition of $V(G)$ of $G = L(CNC_k[n])$

d_v	2	3	4
Number of vertices	k	2kn	7k

Table 3: Edge partition of edge set of $G = L(CNC_k[n])$

(D_u, D_v)	(2,3)	(3,3)	(3,4)	(4,4)
Number of edges	2k	k(2n-1)	2kn	3kn ²

Now from the definition of the M-polynomial,

$$\begin{aligned}
 M(L(CNC_k[n]); x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\
 &= \sum_{2 \leq 3} m_{23} x^2 y^3 + \sum_{3 \leq 3} m_{33} x^3 y^3 + \sum_{3 \leq 4} m_{34} x^3 y^4 + \sum_{4 \leq 4} m_{44} x^4 y^4 \\
 &= \sum_{uv \in E_1(L(CNC_k[n]))} m_{23} x^2 y^3 + \sum_{uv \in E_2(L(CNC_k[n]))} m_{33} x^3 y^3 \\
 &\quad + \sum_{uv \in E_3(L(CNC_k[n]))} m_{34} x^3 y^4 + \sum_{uv \in E_4(L(CNC_k[n]))} m_{44} x^4 y^4 \\
 &= |E_1(L(CNC_k[n]))| x^2 y^3 + |E_2(L(CNC_k[n]))| x^3 y^3 \\
 &\quad + |E_3(L(CNC_k[n]))| x^3 y^4 + |E_4(L(CNC_k[n]))| x^4 y^4 \\
 &= 2kx^2 y^3 + k(2n-1)x^3 y^3 + 2knx^3 y^4 + 3kn^2 x^4 y^4.
 \end{aligned}$$

Figure 4 is plotted using Maple 13. This suggests that the values obtained by M-polynomial increase rapidly along the corners.

Now we compute some degree-based topological indices of nanocones from this M-polynomial.

Proposition 2

Let $G = L(CNC_k[n])$ be the line graph of the carbon nanocones. Then,

- $M_1(L(CNC_k[n])) = 24kn^2 + 26kn + 4k.$
- $M_2(L(CNC_k[n])) = 48kn^2 + 42kn + 3k.$
- ${}^m M_2(L(CNC_k[n])) = (3/16)kn^2 + (7/18)kn + (2/9)k.$
- $RR_\alpha(L(CNC_k[n])) = 3 \times 16^\alpha kn^2 + 2 \times 9^\alpha kn + 2 \times 12^\alpha kn + 2 \times 6^\alpha k - 9^\alpha k.$

$$5. R_\alpha(L(CNC_k[n])) = k \left(\frac{3}{16^\alpha} n^2 + \frac{2}{9^\alpha} n + \frac{2}{12^\alpha} n - \frac{1}{9^\alpha} + \frac{2}{6^\alpha} \right).$$

$$6. SSD(L(CNC_k[n])) = 6kn^2 + \frac{49}{6}kn + \frac{7}{3}k.$$

$$7. H(L(CNC_k[n])) = \frac{3}{8}kn^2 + \frac{13}{21}kn + \frac{7}{30}k.$$

$$8. I(L(CNC_k[n])) = 6kn^2 + \frac{45}{7}kn + \frac{9}{10}k.$$

$$9. A(L(CNC_k[n])) = 2048kn^2 + \frac{10557}{10}kn - \frac{153}{4}k.$$

Proof

Let,

$$M(L(CNC_k[n]); x, y) = f(x, y) = 2kx^2y^3 + k(2n-1)x^3y^3 + 2knx^3y^4 + 3kn^2x^4y^4.$$

Then,

$$D_x(f(x, y)) = 4kx^2y^3 + 3k(2n-1)x^3y^3 + 6knx^3y^4 + 12kn^2x^4y^4,$$

$$D_y(f(x, y)) = 6kx^2y^3 + 3k(2n-1)x^3y^3 + 8knx^3y^4 + 12kn^2x^4y^4,$$

$$(D_y D_x)(f(x, y)) = 12kx^2y^3 + 9k(2n-1)x^3y^3 + 24knx^3y^4 + 48kn^2x^4y^4,$$

$$S_x S_y(f(x, y)) = \frac{1}{3}kx^2y^3 + \frac{1}{9}k(2n-1)x^3y^3 + \frac{1}{6}knx^3y^4 + \frac{3}{16}kn^2x^4y^4,$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 2 \times 6^\alpha kx^2y^3 + 9^\alpha k(2n-1)x^3y^3 + 2 \times 12^\alpha knx^3y^4 + 3 \times 16^\alpha kn^2x^4y^4,$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = \frac{2}{6^\alpha}kx^2y^3 + \frac{1}{9^\alpha}k(2n-1)x^3y^3 + \frac{2}{12^\alpha}knx^3y^4 + \frac{3}{16^\alpha}kn^2x^4y^4,$$

$$S_y D_x(f(x, y)) = \frac{4}{3}kx^2y^3 + k(2n-1)x^3y^3 + \frac{3}{2}knx^3y^4 + 3kn^2x^4y^4,$$

$$S_x D_y(f(x, y)) = 3kx^2y^3 + k(2n-1)x^3y^3 + \frac{8}{3}knx^3y^4 + 3kn^2x^4y^4,$$

$$S_x J f(x, y) = \frac{2}{5}kx^5 + \frac{1}{6}k(2n-1)x^6 + \frac{2}{7}knx^7 + \frac{3}{8}kn^2x^8,$$

$$S_x J D_x D_y(f(x, y)) = \frac{12}{5}kx^5 + \frac{3}{2}k(2n-1)x^6 + \frac{24}{7}knx^7 + 6kn^2x^8,$$

$$S_x^3 Q_2 J D_x^3 D_y^3 f(x, y) = \frac{2 \times 6^3}{3}kx^3 + \frac{9^3}{4}k(2n-1)x^4 + \frac{2 \times 12^3}{5}knx^5 + \frac{16^3}{2}kn^2x^6.$$

Now from Table 1,

$$1. M_1(L(CNC_k[n])) = (D_x + D_y)(f(x, y)) \Big|_{x=y=1} \quad 24 \quad 26 \quad 4 = 24kn^2 + 26kn + 4k.$$

$$2. M_2(L(CNC_k[n])) = D_x D_y(f(x, y)) \Big|_{x=y=1} = 48kn^2 + 42kn + 3k.$$

$$3. {}^m M_2(L(CNC_k[n])) = S_x S_y(f(x, y)) \Big|_{x=y=1} = (3/16)kn^2 + (7/18)kn + (2/9)k.$$

$$4. R_\alpha(L(CNC_k[n])) = D_x^\alpha D_y^\alpha(f(x, y)) \Big|_{x=y=1} \quad 3 \quad 16 \quad 2 \quad 9 = 3 \times 16^\alpha kn^2 + 2 \times 9^\alpha kn + 2 \times 12^\alpha kn + 2 \times 6^\alpha k - 9^\alpha k.$$

$$5. RR_\alpha(L(CNC_k[n])) = S_x^\alpha S_y^\alpha(f(x, y)) \Big|_{x=y=1} = k \left(\frac{3}{16^\alpha} n^2 + \frac{2}{9^\alpha} n + \frac{2}{12^\alpha} n - \frac{1}{9^\alpha} + \frac{2}{6^\alpha} \right).$$

$$6. SSD(L(CNC_k[n])) = (S_y D_x + S_x D_y)(f(x, y)) \Big|_{x=y=1}$$

$$= 6kn^2 + \frac{49}{6}kn + \frac{7}{3}k.$$

$$7. H(L(CNC_k[n])) = 2S_x J(f(x, y)) \Big|_{x=1} = \frac{3}{8}kn^2$$

$$+ \frac{13}{21}kn + \frac{7}{30}k.$$

$$8. I(L(CNC_k[n])) = S_x J D_x D_y(f(x, y)) \Big|_{x=1}$$

$$= 6kn^2 + \frac{45}{7}kn + \frac{9}{10}k.$$

$$9. A(L(CNC_k[n])) = S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) \Big|_{x=1} \quad 2048$$

$$= 2048kn^2 + \frac{10557}{10}kn - \frac{153}{4}k.$$

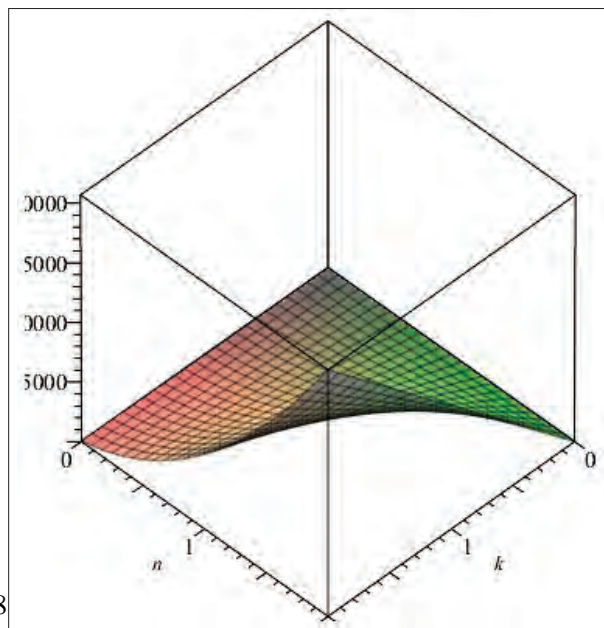


Figure 5: 3D plot of augmented Zagreb index

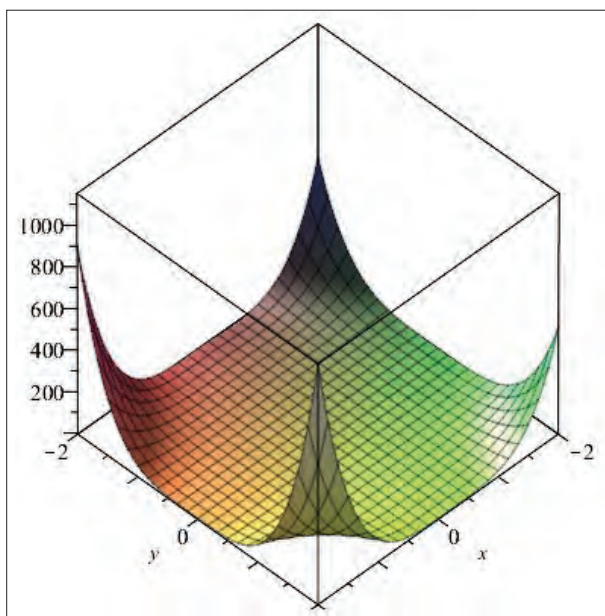


Figure 4: The plot of the M-polynomial of the line graph of carbon nanocones

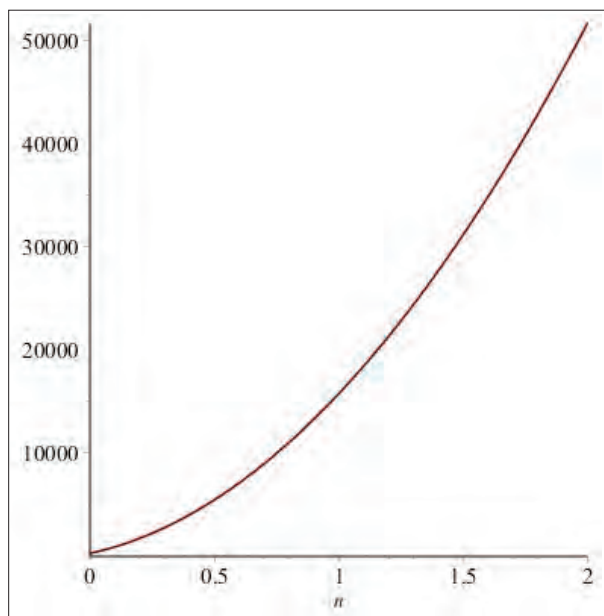


Figure 6: The graph of augmented Zagreb index for k=5

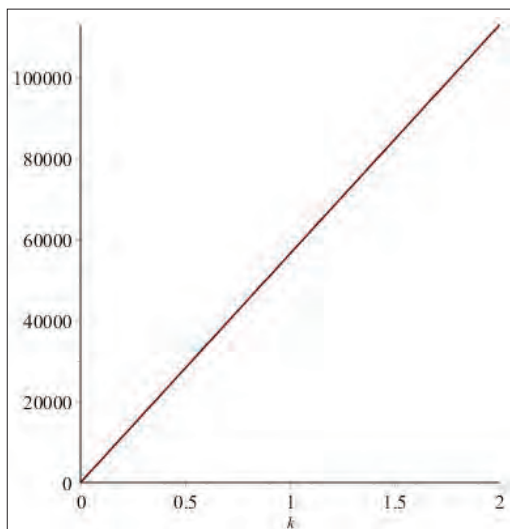


Figure 7: The graph of augmented Zagreb index for $n=5$

CONCLUSION

In this article, we computed general forms of M-polynomials of $L(CNC_k[n])$ for all n and k . This polynomial gives a thorough insight about topological indices and their dependence on the molecular structure of $L(CNC_k[n])$. These indices are actually, experimentally correlated with many properties. All topological indices calculated depend similarly on k and n . Figure 5 is the surface associated to topological index, whereas Figure 6 shows that topological indices are quadratically related with n , but are linearly related with k as Figure 7 suggests.

We pose an open problem to compute the Wiener and other distance-based indices of carbon general nanocones and its line graph. Although some partial results are available for one particular subclass of these nanocones it will be interesting to see how the reactivity is affected by the change in sizes of general nanocones and their Wiener indices.

Acknowledgements

This research is supported by funds from Dong-A University, South Korea.

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