The $M$-Polynomials and Topological Indices of Toroidal Polyhex Network

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Abstract
The $M$-polynomial of different molecular structures helps us to calculate many topological indices. A topological index of graph $G$ is

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a numerical parameter related to $G$ which characterizes its molecular topology. The theoretical properties of the chemical compounds and their molecular topological indices such as the Zagreb indices, Randić index, Symmetric division index, Harmonic index, Inverse sum index, Augmented Zagreb index, etc are correlated. In this report, we computed closed form of the $M$-polynomial of toroidal polyhex network. From the $M$-polynomial we recover some degree-based topological indices for this network.

**Mathematics Subject Classification:** 05C90

**Keywords:** $M$-polynomial, topological index, network

## 1 Introduction

In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges respectively. A graph $G(V, E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there exist a connection between any pair of vertices in $G$. A network is simply a connected graph having no multiple edges and loops. The degree of a vertex is the number of vertices which are connected to that fixed vertex by the edges. In a chemical graph, the degree of any vertex is at most 4. The distance between two vertices $u$ and $v$ is denoted as $d(u, v)$ and is the length of shortest path between $u$ and $v$ in graph $G$. The number of vertices of $G$, adjacent to a given vertex $v$, is the “degree” of this vertex, and will be denoted by $d_v$. The concept of degree is somewhat closely related to the concept of valence in chemistry. For details on bases of graph theory, any standard text such as [29] can be of great help.

Cheminformatics is another emerging field in which quantitative structure-activity and structure-property relationships predict the biological activities and properties of nanomaterial. In these studies, some Physico-chemical properties and topological indices are used to predict bioactivity of the chemical compounds see [28]. Algebraic polynomials have also useful applications in chemistry such as Hosoya polynomial (also called Wiener polynomial) [15] which play a vital role in determining distance-based topological indices. Among other algebraic polynomials, the $M$-polynomial [8] introduced in 2015, plays the same role in determining the closed form of many degree-based topological indices [1, 22–25]. The main advantage of the $M$-polynomial is the wealth of information that it contains about degree-based graph invariants.

In this article, we compute closed form of some degree-based topological indices of toroidal polyhex network by using the $M$-polynomial.
Definition 1.1. ([8]) 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

$$\delta = \min \{d_v : v \in V(G)\}, \quad \Delta = \max \{d_v : v \in V(G)\},$$

and $m_{ij}(G)$ the number of edges $vu \in E(G)$ such that $\{d_v, d_u\} = \{i, j\}$.

Weiner [30] in 1947 approximated the boiling point of alkanes as $\alpha W(G) + \beta P_3 + \gamma$, where $\alpha$, $\beta$ and $\gamma$ are empirical constants, $W(G)$ is the Wiener index and $P_3$ is the number of paths of length 3 in $G$. Thus Weiner laid the foundation of topological index which is also known as connectivity index. A lot of chemical experiments require determining the chemical properties of emerging nanotubes and nanomaterials. Chemical-based experiments reveal that out of more than 140 topological indices, no single index in strong enough to determine many physico-chemical properties, although, in combination, these topological indices can do this to some extent. The Wiener index is originally the first and most studied topological index, see for details [10]. Randić index denoted by $R^{-1/2}(G)$ and introduced by Randić [27] in 1975 is also one of the oldest topological indexes. The Randić index is defined as $R^{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$.

In 1998, working independently, Bollobás and Erdős [6] and Amić et al. [2] proposed the generalized Randić index and has been studied extensively by both chemist and mathematicians and many mathematical properties of this index have been discussed. For a detailed survey we refer the book [19].

The general Randić index is defined as

$$R_{\alpha}(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^{\alpha}},$$

and the inverse Randić index is defined as

$$RR_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}.$$

Obviously $R^{-1/2}(G)$ is the particular case of $R_{\alpha}(G)$ when $\alpha = -\frac{1}{2}$. The suitability of the Randić index for drug design was immediately recognized, 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 [16] introduced 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. For detail about these indices we refer [26] to the readers.

Both the first Zagreb index and the second Zagreb index give greater weights to the inner vertices and edges, and smaller weights to outer vertices and edges which oppose intuitive reasoning [21]. For a simple connected graph \( G \), the second modified Zagreb index is defined as

\[ M_2^m(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)}. \]

The symmetric division index (SDD) is one of the 148 discrete Adriatic indices is a good predictor of the total surface area for polychlorobiphenyls, see [14]. The Symmetric division index of a connected graph \( G \), 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 Randić index is the harmonic index defined as

\[ H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}. \]

As far as we know, this index first appeared in [12].

The inverse sum-index, is the descriptor that was selected in [3] as a significant predictor of total surface area of octane isomers and for which the extremal graphs obtained with the help of mathematical chemistry have a particularly simple and elegant structure. The inverse sum-index is defined as:

\[ I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{(d_u + d_v)}. \]

The augmented Zagreb index of \( G \) proposed by Furtula et al. [13] is defined as

\[ A(G) = \sum_{uv \in E(G)} \left\{ \frac{d_u d_v}{(d_u + d_v - 2)} \right\}^3. \]

This graph invariant has proven to be a valuable predictive index in the study of the heat of formation in octanes and heptanes (see [13]), whose prediction power is better than atom-bond connectivity index (please refer to [7] for its research background). Moreover, the tight upper and lower bounds for the augmented Zagreb index of chemical trees, and the trees with minimal augmented Zagreb index were obtained in [13].
The following Table 1 relates some well-known degree-based topological indices with the $M$-polynomial [8].

<table>
<thead>
<tr>
<th>Topological Index</th>
<th>Derivation from $M(G; x, y)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Zagreb Index</td>
<td>$(D_x + D_y)(M(G; x, y))_{x=y=1}$</td>
</tr>
<tr>
<td>Second Zagreb Index</td>
<td>$(D_xD_y)(M(G; x, y))_{x=y=1}$</td>
</tr>
<tr>
<td>Modified Second Zagreb Index</td>
<td>$(S_xS_y)(M(G; x, y))_{x=y=1}$</td>
</tr>
<tr>
<td>Randić Index</td>
<td>$(D_x^2D_y^2)(M(G; x, y))_{x=y=1}$</td>
</tr>
<tr>
<td>Inverse Randić Index</td>
<td>$(S_x^aS_y^a)(M(G; x, y))_{x=y=1}$</td>
</tr>
<tr>
<td>Symmetric Division Index</td>
<td>$(D_xS_y + S_xD_y)(M(G; x, y))_{x=y=1}$</td>
</tr>
<tr>
<td>Harmonic Index</td>
<td>$2S_xJ(M(G; x, y))_{x=1}$</td>
</tr>
<tr>
<td>Inverse sum Index</td>
<td>$S_xJD_xD_y(M(G; x, y))_{x=1}$</td>
</tr>
<tr>
<td>Augumented Zagreb Index</td>
<td>$S_x^aQ^{-2}JD_x^2D_y^2(M(G; x, y))_{x=1}$</td>
</tr>
</tbody>
</table>

In Table 1,

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

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

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

In this article, we computed closed form of the $M$-polynomial for the toroidal polyhex network. We also computed some degree-based topological indices of this network.

## 2 Computational aspects of toroidal polyhex network

The discovery of the fullerene molecules has stimulated many interests in other possibilities for carbons. Many properties of fullerenes can be studied using mathematical tools such as graph theory. A fullerene can be represented by a trivalent graph on a closed surface with pentagonal and hexagonal faces, such that its vertices are carbon atoms of the molecule. Two vertices are adjacent if there is a bond between corresponding atoms. In [9], authors considered fullerenes' extension to other closed surfaces and showed that only four surfaces, sphere, torus, Klein bottle and projective (elliptic) plane, are possible. The spherical and elliptic fullerenes have 12 and 6 pentagons respectively. There are no pentagons in the toroidal’s and the Klein bottle’s fullerenes [18].

A toroidal fullerene (toroidal polyhex), obtained from 3D Polyhex Torus Figure 1, is a cubic bipartite graph embedded on the torus such that each face...
is a hexagon. The torus is a closed surface that can carry the graphs of the toroidal polyhex in which all faces are hexagons and the degree of all vertices is 3. The optical and vibrational properties of toroidal carbon nanotubes can be found in [5]. There have appeared a few works in the enumeration of perfect matchings of toroidal polyhexes by applying various techniques, such as transfer-matrix and permanent of the adjacency matrix. Ye et al. [31] have studied a k-resonance of toroidal polyhexes. Classifications of all possible structures of fullerene Cayley graphs is given by Kang [17]. The atom-bond connectivity index and geometric-arithmetic index of the toroidal polyhex are computed by Bača et al. [4]. In [20], authors computed distance-based topological indices of eight infinite sequences of 3-generalized fullerenes. In [11], authors presented a new extension of the generalized topological indices approach to represent topological indices in a unified way.

![Figure 1. Polyhex torus](image1)

First identify two lateral sides of $P^n_m$ to form a cylinder, and finally identify the top and bottom sides of $P^n_m$ at their corresponding points, see Figure 2. From this we get a toroidal polyhex $H_{(m,n)}$ with $mn$ hexagons.

![Figure 2. 2D-lattice graph of the toroidal polyhex](image2)
The set of vertices of the toroidal polyhex is

\[ V(H_{(m,n)}) = \{v^i_j, v^i_j : 0 \leq i \leq n - 1, 0 \leq j \leq m - 1\}. \]

The set of edges of the toroidal polyhex is splitted into mutually disjoint subsets such that for even \( i \) such that \( 0 \leq i \leq n - 2 \), we have \( A_i = \{v^i_j, v^i_{j+1} : 0 \leq j \leq m-1\} \) and \( A'_i = \{v^i_{j+1}, v^i_j : 0 \leq j \leq m-1\} \). For odd \( 1 \leq i \leq n - 1 \), we have \( A_i = \{v^i_j, v^i_{j+1} : 0 \leq j \leq m-1\} \) and \( B_i = \{v^i_j, v^i_{j+1} : 0 \leq j \leq m-1\} \). For \( 0 \leq i \leq n - 1 \), we have \( C_i = \{v^i_j, v^i_{j+1} : 0 \leq j \leq m-1\} \), where \( i \) is taken modulo \( n \) and \( j \) is taken modulo \( m \). Hence \( E(H_{(m,n)}) = \bigcup_{i=0}^{n-1}(A_{2i} \cup A'_{2i} \cup B_{2i+1} \cup B'_{2i+1}) \bigcup_{i=0}^{n-1} C_i \).

We can easily observe from Figure 2 that the number of vertices in \( H_{(m,n)} \) are \( 2mn \) and the number of edges in \( H_{(m,n)} \) are \( 3mn \).

**Theorem 2.1.** Let \( H_{(m,n)} \) be the toroidal polyhex. Then the M-polynomial of \( H_{(m,n)} \) is

\[ M(H_{(m,n)}, x, y) = 3mnx^3y^3. \]

**Proof.** Let \( H_{(m,n)} \) be the octagonal network. There is only one type of edges in toroidal polyhex based on degrees of end vertices of each edge. The edge partition \( E_1(H_{(m,n)}) \) contains \( 3mn \) edges uv, where \( d_u = d_v = 3 \). From definition of the M-polynomial

\[ M(H_{(m,n)}, x, y) = \sum_{i\leq j} m_{ij}x^iy^j = \sum_{3 \leq 3} m_{33}x^3y^3 \]

\[ = \sum_{uv \in E_1(H_{(m,n)})} m_{33}x^3y^3 = 3mnx^3y^3. \]

This completes the proof. \( \square \)

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

**Proposition 2.2.** Let \( H_{(m,n)} \) be the toroidal polyhex. Then

1. \( M_1(H_{(m,n)}) = 18mn \).
2. \( M_2(H_{(m,n)}) = 27mn \).
3. \( M_3^m(H_{(m,n)}) = \frac{mn}{3} \).
4. \( R_\alpha(H_{(m,n)}) = 3^{2\alpha+1}mn \).
5. \( R_\alpha(H_{(m,n)}) = 3^{1-2\alpha}mn \).
6. \( SSD(H_{(m,n)}) = 6mn \).
7. \( H(H_{(m,n)}) = mn \).
8. \( I(H_{(m,n)}) = \frac{9mn}{2} \).
9. \( A(H_{(m,n)}) = \frac{2178}{64}mn \).
Proof. Let $M(H_{m,n}, x, y) = f(x, y) = 3mnx^3y^3$. Then

\begin{align*} 
D_x f(x, y) &= 9mnx^3y^3, \\
D_y f(x, y) &= 9mnx^3y^3, \\
D_y D_x f(x, y) &= 27mnx^3y^3, \\
S_x S_y (f(x, y)) &= \frac{1}{3}mnx^3y^3, \\
D_y^2 S_y^2 (f(x, y)) &= 3^{2\alpha+1}mnx^3y^3, \\
S_x^2 S_y^2 (f(x, y)) &= \frac{1}{3^{2\alpha+1}}mnx^3y^3, \\
S_y D_x (f(x, y)) &= 3mnx^3y^3, \\
S_x D_y (f(x, y)) &= 3mnx^3y^3, \\
S_x J (f(x, y)) &= \frac{1}{2}mnx^6, \\
S_x JD_x D_y (f(x, y)) &= \frac{9}{2}mnx^6, \\
S_x^3 Q_{-2} JD_x^2 D_y^2 (f(x, y)) &= \frac{81}{127}mnx^4. 
\end{align*}

From Table 1, 1. $M_1(H_{m,n}) = (D_x + D_y) f(x, y) |_{x=y=1} = 18mn$.
2. $M_2(H_{m,n}) = D_x + D_y f(x, y) |_{x=y=1} = 27mn$.
3. $M_2^m(H_{m,n}) = S_x S_y f(x, y) |_{x=y=1} = \frac{mn}{3}$.
4. $R_2(H_{m,n}) = D_x^2 D_y^2 f(x, y) |_{x=y=1} = 3^{2\alpha+1}mn$.
5. $R_2(H_{m,n}) = S_x^2 S_y^2 f(x, y) |_{x=y=1} = 3^{2\alpha+1}mn$.
6. $SSD(H_{m,n}) = (S_y D_x + S_x D_y f(x, y)) |_{x=y=1} = 6mn$.
7. $H(H_{m,n}) = 2S_x J(f(x, y)) |_{x=1} = mn$.
8. $I(H_{m,n}) = S_x JD_x D_y (f(x, y)) |_{x=1} = \frac{9mn}{2}$.
9. $A(H_{m,n}) = S_x^3 Q_{-2} JD_x^2 D_y^2 (f(x, y)) = \frac{2187}{64}mn$.

This completed the proof. \qed

3 Conclusions

In this article we compute many topological indices for generalized prism and toroidal polyhex networks. At first we give general closed form of $M$-polynomial of this network and then recover many degree-based topological indices out of it. These results can play a vital rule in preparation of new drugs.

References


Received: February 15, 2017; Published: March 16, 2017