

Research Article

New Degree-Based Topological Indices of Toroidal Polyhex Graph by Means of M-Polynomial

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Graph theory is the principal field of mathematics. In this manuscript, we have discussed the toroidal polyhex graph. Some new indices such as reduced reciprocal randic, arithmetic geometric, SK, SK₁, SK₂ indices, First Zagreb, the general sum-connectivity, SCI₁, and the forgotten index have been used. We have computed the closed form of topological indices of toroidal polyhex graph via M-Polynomial.

1. Introduction

Graph theory in mathematics means the study of graphs. Graphs are one of the prime objects of study in discrete mathematics. The graph appears as a set of vertices (nodes or points) connected by edges (arcs or lines). Graphs are mathematical structures of the diagram formed by using model pairwise relation between objects. They are found on road maps and constellations when constructing schemes and drawing. Graphs underlie many computer programs that make modern communication and technological processes possible. A chemical graph theory is the mixture of two subjects' chemistry and mathematics. The chemical graph is the topological type of mathematical chemistry [1] which declares in a graph to mathematical modeling of the chemical event. Sometimes mathematical chemistry is also called computer chemistry [2]. Chemical graph is concerned with searching the topological indices associated with the properties of chemical molecules [3].

A graph $G(V; E)$ with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a connection between any pair of vertices in G . A network directly connected graph having no multiple edges and loops. The degree of a vertex is several vertices that are fastened to the connected vertex by the edges.

The first topological index was used by Wiener [4]. Topological indices work for the success of the quantitative activity and other properties of a molecule that correlate with chemical structure. The connection between atoms shown by various types of topological indices give a good guess of different chemical properties of the chemical compound such as boiling point, the heat of formation, evaporation, surface tension, and vapor pressure.

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compound such as boiling point, the heat of formation, evaporation, surface tension, and vapor pressure. The topological indices are computed via M-polynomial. Several works are done in this area [6–8].

1.1. Reduced Reciprocal Randic Index

$$\text{RRR}(G) = \sum_{jk \in E(G)} \sqrt{(d_j - 1)(d_k - 1)}. \quad (1)$$

In 2015 [9], Gutman and Furtula introduced a reduced reciprocal index. The reduced reciprocal randic (RRR) index is a molecular structure descriptor (or more precisely, a topological index), handy for a divine level of enthalpy creation and usual boiling point of isomeric octanes.

1.2. Arithmetic Geometric Index

$$\text{AG}_1(G) = \sum_{jk \in E(G)} \frac{d_j + d_k}{2\sqrt{d_j \cdot d_k}}. \quad (2)$$

In 2016 [8], Deutsch and Klawzar used the arithmetic geometric index.

SK , SK_1 , and SK_2 indices are denied as

$$\begin{aligned} \text{SK}(G) &= \sum_{jk \in E(G)} \frac{d_j + d_k}{2}, \\ \text{SK}_1(G) &= \sum_{jk \in E(G)} \frac{d_j \cdot d_k}{2}, \\ \text{SK}_2(G) &= \sum_{jk \in E(G)} \left(\frac{d_j \cdot d_k}{2} \right)^2. \end{aligned} \quad (3)$$

In 2016 [10], Shegehalli and Kanabur also used SK , SK_1 , and SK_2 indices.

1.3. First Zagrab Index. First Zagrab index was used in 2014 [11].

$$\text{EM}_1(G) = \sum_{jk \in E(G)} (d_{jk})^2. \quad (4)$$

1.4. General Sum-Connectivity Index. Firstly, general sum-connectivity index was used by Du et al. in 2011 [12].

$$\text{SCI}(G) = \sum_{jk \in E(G)} \frac{1}{\sqrt{d_j + d_k}}. \quad (5)$$

1.5. SCI_λ Index. Also, SCI_λ was used by Du et al. in 2011 [12].

$$\text{SCI}_\lambda = \sum_{jk \in E(G)} (d_j + d_k)^\lambda. \quad (6)$$

1.6. Forgotten Index. Gutman and Furtula introduced forgotten index in 2015 [9].

$$F(G) = \sum_{jk \in E(G)} (d_j^2 + d_k^2). \quad (7)$$

Definition 1. The M-polynomial is firstly used in 2015 [8] and is determined as follows:

$$M(G, x, y) = \sum_{\rho \leq j \leq k \leq \phi} m_{ij}(G) x^j y^k, \quad (8)$$

where $\rho = \max\{d_v : v \in V(G)\}$, $\phi = \min\{d_v : v \in V(G)\}$, and $m_{jk}(G)$ is the total number of edges $vu \in E(G)$ where $\{d_v, d_u\} = \{j, k\}$.

In last few years, M-polynomial of several graphs is invented [5, 13–16]. In Table 1, degree-dependent topological indices via M-polynomial are provided where

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

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

$$Jg(x, y) = g(x, x),$$

$$Q_{x(\alpha)} g(x, y) x^\alpha g(x, y),$$

$$D_x^{(1/2)}(g(x, y)) = \sqrt{x \frac{\partial(g(x, y))}{\partial x}} \cdot \sqrt{g(x, y)}, \quad (9)$$

$$D_y^{(1/2)}(g(x, y)) = \sqrt{y \frac{\partial(g(x, y))}{\partial y}} \cdot \sqrt{g(x, y)},$$

$$S_x^{(1/2)}(g(x, y)) = \sqrt{\int_0^x \frac{g(t, y)}{t} dt} \cdot \sqrt{g(x, y)},$$

$$S_y^{(1/2)}(g(x, y)) = \sqrt{\int_0^y \frac{g(x, t)}{t} dt} \cdot \sqrt{g(x, y)}.$$

2. Toroidal Polyhex Network

Fullerene was published in 1985. New forms of the element carbon (C) were established by Robert C, Richard E. Smalley, and Sir Harold W. K. Fullerene is an allotrope form of carbon whose molecules exist in carbon atoms attached by single and double bonds that can be the form of closed mesh or slightly closed mesh, with a fused ring of five to seven atoms. These molecules may be hollow spheres, ellipsoid, tube, and many more shapes and sizes.

Let $H_{\{m,n\}}$ be the toroidal polyhex as shown in Figure 1. The M-polynomial of $H_{\{m,n\}}$ which have been computed in [17] is given as $M(H_{\{m,n\}}, x, y) = 3mnx^3y^3$. The graph of 3D plot of M-polynomial of toroidal polyhex network $m = n = 2$ is shown in Figure 2.

TABLE 1: Degree-dependent topological indices via M-polynomial.

Topological index	Derivation from $M(G; x, y)$
Reduced reciprocal randic	$RRR[G] = D_x^{(1/2)}D_y^{(1/2)}Q_{y(-1)}Q_{x(-1)}[g(x, y)]_{x=y=1}$
Arithmetic geometric index	$AG_1[G] = (1/2)D_xJS_x^{(1/2)}S_y^{(1/2)}[g(x, y)]_{x=1}$
SK index	$SK[G] = (1/2)(D_x + D_y)[g(x, y)]_{x=y=1}$
SK_1 index	$SK_1[G] = (1/2)(D_xD_y)[g(x, y)]_{x=y=1}$
SK_2 index	$SK_2[G] = (1/4)D_x^2J[g(x, y)]_{x=y=1}$
First Zagrab index	$EM_1[G] = D_x^2Q_{x(-2)}J[g(x, y)]_{x=1}$
General sum-connectivity index	$SCI[G] = S_x^{(1/2)}J[g(x, y)]_{x=1}$
SCI_λ index	$SCI_\lambda[G] = D_x^\lambda J[g(x, y)]_{x=1}$
Forgotten index	$F[G] = (D_x^2 + D_y^2)[g(x, y)]_{x=1}$



FIGURE 1: The toroidal polyhex.

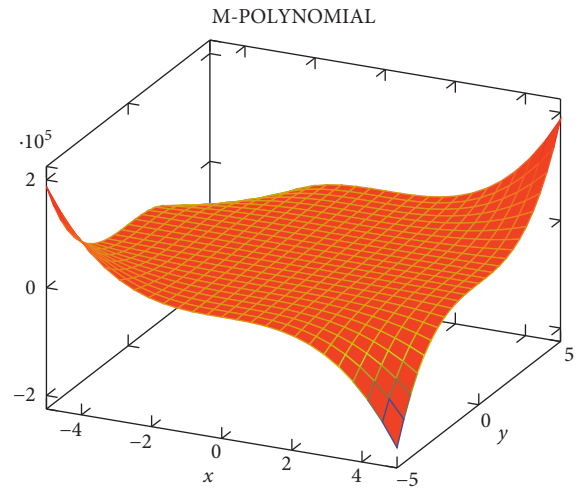


FIGURE 2: Plot of M-polynomial of toroidal polyhex.

3. Topological Indices of Toroidal Polyhedral Network

Theorem 1. Let $H_{\{m,n\}}$ be the toroidal polyhedral.

$$M(H_{\{m,n\}}, x, y) = 3mnx^3y^3. \tag{10}$$

Then,

- (i) $RRR(H_{\{m,n\}}) = 6mn$
- (ii) $AG_1(H_{\{m,n\}}) = 3mn$
- (iii) $SK(H_{\{m,n\}}) = 9mn$

- (iv) $SK_1(H_{\{m,n\}}) = (27/2)mn$
- (v) $SK_2(H_{\{m,n\}}) = 27mn$
- (vi) $EM_1(H_{\{m,n\}}) = 48mn$
- (vii) $SCI(H_{\{m,n\}}) = (\sqrt{3}/\sqrt{2})mn$
- (viii) $SCI_\lambda(H_{\{m,n\}}) = 18^\lambda mn$
- (ix) $F(H_{\{m,n\}}) = 54mn$

Proof. Let $M(H_{\{m,n\}}, x, y) = 3mnx^3y^3$.

(1) Reduced reciprocal randic index is as follows:

$$\begin{aligned}
 Q_{x(-1)}g(x, y) &= 3mnx^2y^3, \\
 Q_{y(-1)}Q_{x(-1)}g(x, y) &= 3mn^2y^2, \\
 D_y^{(1/2)}Q_{y(-1)}Q_{x(-1)}g(x, y) &= 3\sqrt{2}mn, \\
 D_x^{(1/2)}D_y^{(1/2)}Q_{y(-1)}Q_{x(-1)}g(x, y) &= 6mnx^2y^2, \\
 RRR(H_{\{m,n\}}) &= D_x^{(1/2)}D_y^{(1/2)}Q_{y(-1)}Q_{x(-1)}[g(x, y)]_{x=1} = 6mn.
 \end{aligned} \tag{11}$$

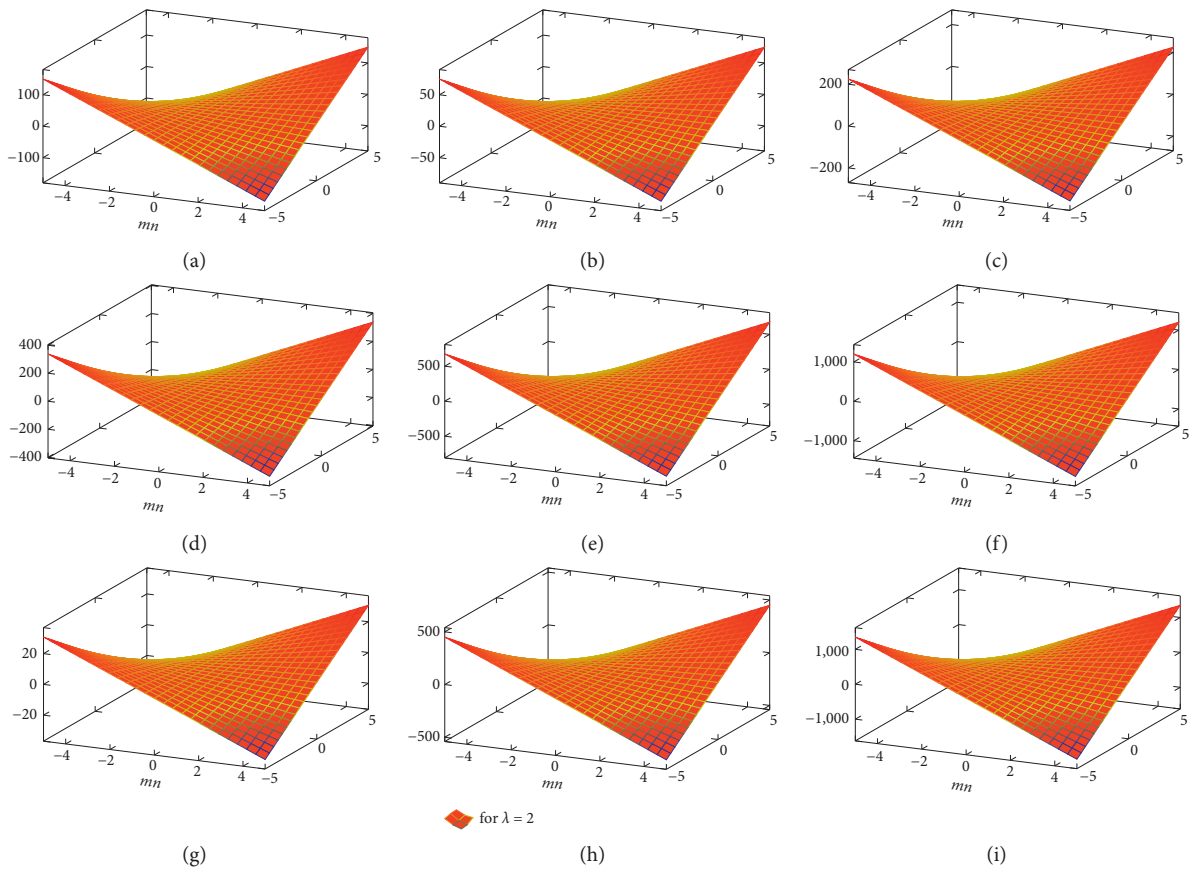


FIGURE 3: The plot of topological indices. (a) Reduced reciprocal randic index. (b) Arithmetic geometric index. (c) SK index. (d) SK₁ index. (e) SK₂ index. (f) First Zagrab index. (g) General sum-connectivity index. (h) SCL_λ index. (i) Forgotten index.

(2) Arithmetic geometric index is as follows:

$$\begin{aligned}
 S_y^{(1/2)}g(x, y) &= \sqrt{3}mnx^3y^3, \\
 S_x^{(1/2)}S_y^{(1/2)}g(x, y) &= mnx^3y^3, \\
 JS_x^{(1/2)}S_y^{(1/2)}g(x, y) &= mnx^6, \\
 D_xJS_x^{(1/2)}S_y^{(1/2)}g(x, y) &= 6mnx^6, \\
 \frac{1}{2}D_xJS_x^{(1/2)}S_y^{(1/2)}g(x, y) &= 3mnx^6, \\
 AG_1(H_{\{m,n\}}) &= \frac{1}{2}D_xJS_x^{(1/2)}S_y^{(1/2)}[g(x, y)]_{x=y=1} \\
 &= 3mn.
 \end{aligned}
 \tag{12}$$

(3) SK index is as follows:

$$\begin{aligned}
 D_xg(x, y) &= 9mnx^3y^3, \\
 D_yg(x, y) &= 9mnx^3y^3, \\
 (D_x + D_y)g(x, y) &= 18mnx^3y^3, \\
 \frac{1}{2}(D_x + D_y)g(x, y) &= 9mnx^3y^3, \\
 SK(H_{\{m,n\}}) &= \frac{1}{2}(D_x + D_y)[g(x, y)]_{x=y=1} = 9mn.
 \end{aligned}
 \tag{13}$$

(4) SK₁ index is as follows:

$$\begin{aligned}
 D_yg(x, y) &= 9mnx^3y^3, \\
 (D_xD_y)g(x, y) &= 27mnx^3y^3, \\
 \frac{1}{2}(D_xD_y)g(x, y) &= \frac{27}{2}mnx^3y^3, \\
 SK_1(H_{\{m,n\}}) &= \frac{1}{2}(D_xD_y)[g(x, y)]_{x=y=1} = \frac{27}{2}mn.
 \end{aligned}
 \tag{14}$$

(5) SK₂ index is as follows:

$$\begin{aligned}
 Jg(x, y) &= 3mnx^6, \\
 D_x^2Jg(x, y) &= 108mnx^6, \\
 \frac{1}{4}D_x^2Jg(x, y) &= 27mnx^6, \\
 SK_2(H_{\{m,n\}}) &= \frac{1}{4}D_x^2J[g(x, y)]_{x=y=1} = 27mn.
 \end{aligned}
 \tag{15}$$

(6) First Zagrab index is as follows:

$$Jg(x, y) = 3mnx^6,$$

$$Q_{x(-2)}Jg(x, y) = 3mnx^4,$$

$$D_x^2 Q_{x(-2)}Jg(x, y) = 48mnx^4,$$

$$EM_1(H_{\{m,n\}}) = D_x^2 Q_{x(-2)}J[g(x, y)]_{x=1} = 48mn. \quad (16)$$

(7) General sum-connectivity index is as follows:

$$Jg(x, y) = 3mnx^6,$$

$$S_x^{(1/2)}Jg(x, y) = \frac{\sqrt{3}}{\sqrt{2}}mnx^6, \quad (17)$$

$$SCI(H_{\{m,n\}}) = S_x^{(1/2)}J[g(x, y)]_{x=1} = \frac{\sqrt{3}}{\sqrt{2}}mn.$$

(8) SCI_λ index is as follows:

$$Jg(x, y) = 3mnx^6,$$

$$D_x^\lambda Jg(x, y) = 18^\lambda mnx^6, \quad (18)$$

$$SCI_\lambda(H_{\{m,n\}}) = D_x^\lambda J[g(x, y)]_{x=1} = 18^\lambda mn.$$

(9) Forgotten index is as follows:

$$D_y^2 g(x, y) = 27mnx^3 y^3,$$

$$D_x^2 g(x, y) = 27mnx^3 y^3,$$

$$(D_x^2 + D_y^2)g(x, y) = 54mnx^3 y^3,$$

$$F(H_{\{m,n\}}) = (D_x^2 + D_y^2)[g(x, y)]_{x=1} = 54mn. \quad (19)$$

□

4. Conclusion

In this article, we assess the toroidal polyhex graph through the degree-based topological indices. The plot of topological indices of toroidal polyhex is given in Figure 3. The M-polynomial calculated the toroidal polyhex that can help us to understand and recover many degree-based topological indices. These topological indices play a vital role.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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