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Computational Analysis of Topological Indices for Hex-derived Networks of Type 3 and Their Subdivisions

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***Abstract*—Topological indices are numerical parameters of a graph that describe its topology and are typically graph invariants. Hex-derived networks are obtained from the hexagonal network and have a variety of applications in the field of pharmacy, electronics and interconnection networks. In this work, we consider two different Hex-derived networks of third type of dimension n with their allied subdivisions. We graphically execute comparative assessments between the M-polynomials and corresponding topological indices of these Hex-derived networks and their associated subdivisions.**

***Index Terms*— Hex-derived network of third type; chain Hex-derived network of third type; subdivision of graph; degree-based topological indices; M-polynomial; graph polynomial.**

I. INTRODUCTION

Let $G = (V, E)$ be a simple, undirected and connected graph, where $V = V(G)$ denotes the vertex set and $E = E(G)$ denotes the edge set. The degree of a vertex $v \in V(G)$ in a graph G counts the number of edges that are incident to v and is symbolized by $d(v)$. A subdivision of a graph is acquired by adding a vertex to an edge of a graph, dividing the edge into two edges [1].

A subfield of mathematical chemistry known as Chemical Graph Theory (CGT) combines graph theory and mathematical modelling of chemical phenomena. The attention of CGT is on the topological indices that have strong relationships with the characteristics of the chemical molecules. Topological indices (in short, we denote it by *TI*) are frequently used to forecast the chemical and physical characteristics of the molecules or to predict biological activity using the QSPR/QSAR (Quantitative Structure-Property/Structure-Activity Relationship) modelling [2]. They can be categorized as distance-dependent, degree-dependent, degree and distance-dependent, and matching-dependent, etc., in accordance with the structural features of the graph.

Several polynomials have evolved in the literature for the estimation of various classes of topological indices. They are Hosoya polynomial [3], M-polynomial [4], Schultz polynomial [5], matching polynomial [6], etc. In 2015, Deutsch and Klavžar proposed the idea of M-polynomial [4] to estimate several degree dependent topological indices. There are numerous articles in the literature [7-11] in which the M-polynomial has been employed to estimate various degree-dependent topological indices.

A. About the Hex-derived Networks and Their Subdivisions

In 1990, Chen et al. produced an addressing scheme and routing and broadcasting algorithms for the hexagonal mesh multiprocessors [12]. The class of networks designed by the planar graphs includes the hexagonal networks. Raj and George developed a new chemical network (known as third type of Hex-derived networks)

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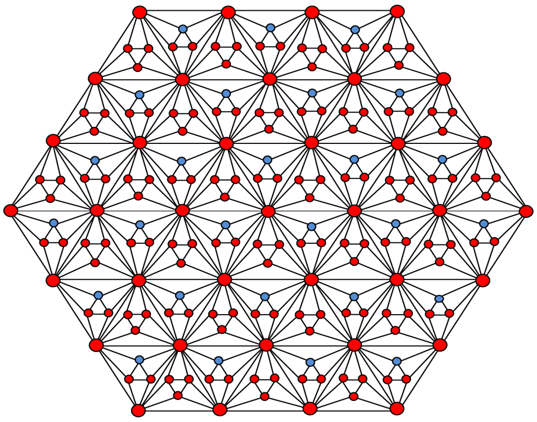
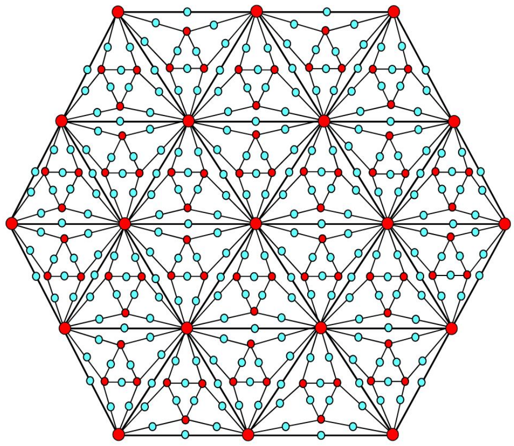
[13] from the hexagonal network of dimension n. Figure 1 contains the graphical representation of the Hex-derived network of third type of dimension n ($HDN3[n]$) and subdivided Hex-derived network of third type of dimension n ($SHDN3[n]$) for some n. See Figure 1(a) for $HDN3[n]$ for $n = 4$ and Figure 1(b) for $SHDN3[n]$ for $n = 3$. For some n, the graphical structure of chain Hex-derived network of third type of dimension n ($CHDN3[n]$) and subdivided chain Hex-derived network of third type of dimension n ($SHDN3[n]$) are included in Figure 2. View Figure 2(a) for $CHDN3[5]$ and Figure 2(b) for $SCHDN3[5]$. For more information about these structures and their properties, please refer to [14-17].

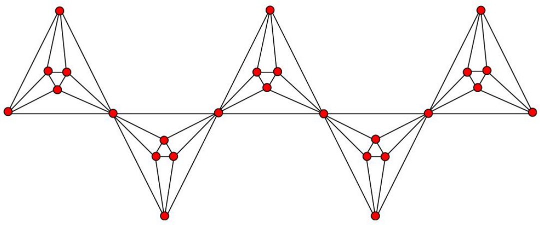


(a) Hex-derived network of third type ($HDN3[4]$)

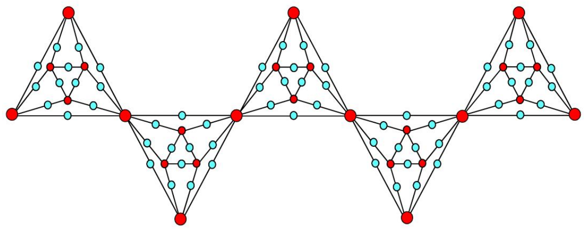


(b) Subdivided Hex-derived network of third type ($SHDN3[3]$)

Figure 1. Structure of Hex-derived and subdivided Hex-derived networks



(a) Chain Hex-derived network of third type (CHDN3[5])



(b) Subdivided chain Hex-derived network of third type (SCHDN3[5])

Figure 2. Structure of chain and subdivided chain Hex-derived networks

B. Our Objectives

In the present work, we have incorporated the $HDN3[n]$, $SHDN3[n]$, $CHDN3[n]$ and $SCHDN3[n]$ networks and executed comparative assessments by taking the M-polynomial expressions and their associated topological indices of these networks. Some necessary existing M-polynomial based results related to the $HDN3[n]$ and $SHDN3[n]$ networks are summarized in Section *C*, from the articles [14, 16]. Also, from [15, 17], we have comprised similar necessary outcomes corresponding to the $CHDN3[n]$ and $SCHDN3[n]$ networks in Section *E*. We perform a comparative study between the existing results corresponding to the M-polynomial and associated topological indices of these Hex-derived networks and their allied subdivisions in Sections *D* and *F*, respectively. We conclude in Section IV.

II. M-POLYNOMIAL BASED COMPARATIVE STUDIES OF $HDN3[n]$ AND $SHDN3[n]$ NETWORKS

This section deals with the M-polynomial based comparative assessment between the $HDN3[n]$ and $SHDN3[n]$ networks. The comparative study on M-polynomials and related topological indices for $HDN3[n]$ and $SHDN3[n]$ networks have been done in Section *D* and the prerequisite results are outlined in Section *C*.

C. Existing Results on $HDN3[n]$ and $SHDN3[n]$ Networks

This section clubbed together the necessary existing results corresponding to the M-polynomials and associated topological indices of the $HDN3[n]$ and $SHDN3[n]$ networks. Theorem 1 contains the M-polynomial expression of the $HDN3[n]$ network, and their corresponding indices are listed in Theorem 2. In a similar manner, Theorem

3 includes the M-polynomial expression of the $SHDN3[n]$ network, and their related topological indices are indexed in Theorem 4.

Theorem 1 ([14]). *Let $HDN3[n]$ denotes the third type of Hex-derived network of dimension n. Then a M-polynomial of the $HDN3[n]$ network, where $n \geq 4$, is*

$$M(HDN3[n]; x, y) = (18n^2 - 36n + 18)x^4y^4 + 24x^4y^7 + (36n - 72)x^4y^{10} + (36n^2 - 108n + 84)x^4y^{18} + 12x^7y^{10} + 6x^7y^{18} + (6n - 18)x^{10}y^{10} + (12n - 24)x^{10}y^{18} + (9n^2 - 33n + 30)x^{18}y^{18}.$$

Theorem 2 ([14]). *Let $HDN3[n]$ represents the third type of Hex-derived network of dimension n. Then*

(i) $M_1(HDN3[n]) = 6(210n^2 - 482n + 275)$,

(ii) $M_2(HDN3[n]) = 12(483n^2 - 1237n + 777)$,

(iii) $mM_2(HDN3[n]) = \frac{119}{72}n^2 - \frac{1907}{675}n + \frac{50921}{37800}$,

(iv) $R_\alpha(HDN3[n]) = 4^{2\alpha}(18n^2 - 36n + 18) + 24 \times 28^\alpha + 40^\alpha(36n - 72) + 72^\alpha(36n^2 - 108n + 84) + 12 \times 70^\alpha + 6 \times 126^\alpha + 10^{2\alpha}(6n - 18) + 180^\alpha(12n - 24) + 18^{2\alpha}(9n^2 - 33n + 30)$,

(v) $RR_\alpha(HDN3[n]) = \frac{1}{4^{2\alpha}}(18n^2 - 36n + 18) + \frac{24}{28^\alpha} + \frac{1}{40^\alpha}(36n - 72) + \frac{1}{72^\alpha}(36n^2 - 108n + 84) + \frac{12}{70^\alpha} + \frac{6}{126^\alpha} + \frac{1}{10^{2\alpha}}(6n - 18) + \frac{1}{180^\alpha}(12n - 24) + \frac{1}{18^{2\alpha}}(9n^2 - 33n + 30)$,

(vi) $SDD(HDN3[n]) = 224n^2 - \frac{1510}{3}n + \frac{30487}{105}$,

(vii) $H(HDN3[n]) = \frac{91}{11}n^2 - \frac{4637}{330}n + \frac{15959}{2550}$,

(viii) $ISI(HDN3[n]) = \frac{2583}{11}n^2 - \frac{5637}{5637}n + \frac{115452}{425}$,

(ix) $AZ(HDN3[n]) = \frac{18072253528}{1842375}n^2 - \frac{9158722597814888}{327863527875}n + \frac{77521944602750189008}{3989115543655125}$.

Theorem 3 ([16]). *Let $SHDN3[n]$ denotes the subdivided Hex-derived network of third type of dimension n. Then the M-polynomial expression of the $SHDN3[n]$ network, where $n \geq 3$, is*

$$M(SHDN3[n]; x, y) = 72(n-1)^2x^2y^4 + 42x^2y^7 + 60(n-2)x^2y^{10} + 18(3n^2 - 9n + 7)x^2y^{18}.$$

Theorem 4 ([16]). *Let $SHDN3[n]$ represents the subdivided Hex-derived network of third type of dimension n. Then*

(i) $M_1(SHDN3[n]) = 18(84n^2 - 188n + 105)$,

(ii) $M_2(SHDN3[n]) = 12(210n^2 - 482n + 275)$,

(iii) $mM_2(SHDN3[n]) = \frac{1}{2}(21n^2 - 39n + 19)$,

(iv) $R_\alpha(SHDN3[n]) = 72 \times 8^\alpha(n-1)^2 + 42 \times 14^\alpha + 60 \times 20^\alpha(n-2) + 18 \times 36^\alpha(3n^2 - 9n + 7)$,

(v) $RR_\alpha(SHDN3[n]) = \frac{72}{8^\alpha}(n-1)^2 + \frac{42}{14^\alpha} + \frac{60}{20^\alpha}(n-2) + \frac{18}{36^\alpha}(3n^2 - 9n + 7)$,

(vi) $SDD(SHDN3[n]) = 672n^2 - 1524n + 863$,

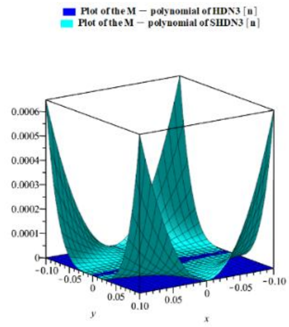
(vii) $H(SHDN3[n]) = \frac{147}{5}n^2 - \frac{271}{5}n + \frac{389}{15}$,

(viii) $ISI(SHDN3[n]) = \frac{966}{5}n^2 - \frac{1918}{5}n + \frac{2822}{15}$,

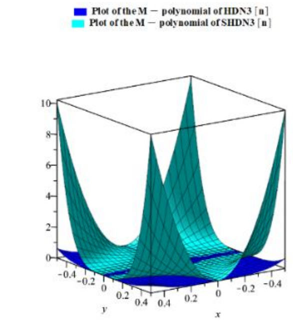
(ix) $AZ(SHDN3[n]) = 48(21n^2 - 41n + 20)$.

D. Main Results: Comparative Analysis Between the $HDN3[n]$ and $SHDN3[n]$ Networks

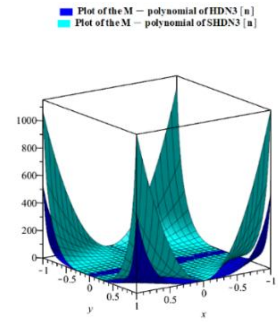
In this section, for the comparative analysis between the $HDN3[n]$ and $SHDN3[n]$ networks, we use the above theorems regarding the M-polynomials and related topological indices of these networks. Using Maple 2020 software environment, we pictorially illustrate (see Figure 3) the expressions of M-polynomial of the $HDN3[n]$ and $SHDN3[n]$ networks for different ranges of x and y in a single framework. We vary the ranges of x and y for the stipulated value of dimension $n = 4$ to observe the behaviour of the comparison plots corresponding to the M-polynomials of the $HDN3[n]$ and $SHDN3[n]$ networks: $-0.1 \leq x \leq 0.1$ in Figure 3(a), $-0.5 \leq x \leq 0.5$ in Figure 3(b), $-1 \leq x \leq 1$ in Figure 3(c), $-1.5 \leq x \leq 1.5$ in Figure 3(d), $-2 \leq x \leq 2$ in Figure 3(e) and $-3 \leq x \leq 3$ in Figure 3(f).



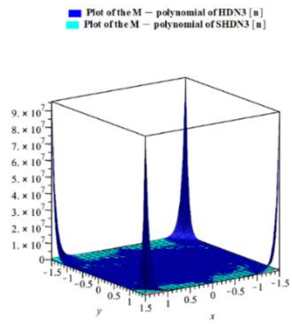
(a) M-polynomial comparison of $HDN3[4]$ and $SHDN3[4]$ networks, where $-0.1 \leq x, y \leq 0.1$



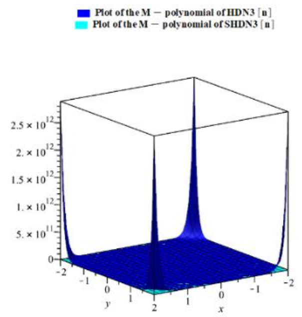
(b) M-polynomial comparison of $HDN3[4]$ and $SHDN3[4]$ networks, where $-0.5 \leq x, y \leq 0.5$



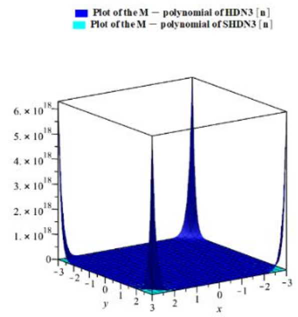
(c) M-polynomial comparison of $HDN3[4]$ and $SHDN3[4]$ networks, where $-1 \leq x, y \leq 1$



(d) M-polynomial comparison of $HDN3[4]$ and $SHDN3[4]$ networks, where $-1.5 \leq x, y \leq 1.5$



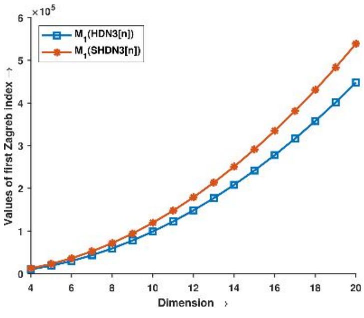
(e) M-polynomial comparison of $HDN3[4]$ and $SHDN3[4]$ networks, where $-2 \leq x, y \leq 2$



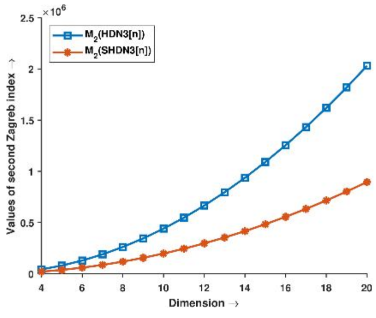
(f) M-polynomial comparison of $HDN3[4]$ and $SHDN3[4]$ networks, where $-3 \leq x, y \leq 3$

Figure 3. A comparative illustration of the M-polynomials of $HDN3[4]$ and $SHDN3[4]$ in different regions of x and y

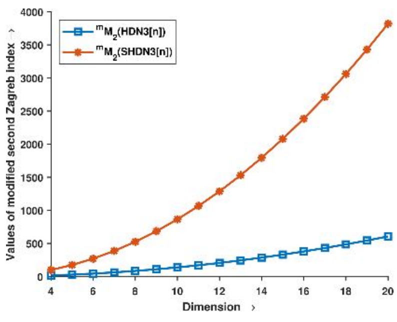
Additionally, using the MATLAB R2019a software, we demonstrate comparison plots of the topological indices (as denoted by TI) of the $HDN3[n]$ and $SHDN3[n]$ networks in Figure 4. Throughout the evaluation of Figure 4, we acquire that $TI(HDN3[n]) \geq TI(SHDN3[n])$ for the second Zagreb index (see Figure 4(b)), inverse sum (indeg) index (see Figure 4(h)) and augmented Zagreb index (see Figure 4(i)), whereas for the first Zagreb index (see Figure 4(a)), modified second Zagreb index (see Figure 4(c)), general Randić index (see Figure 4(d)), symmetric division (deg) index (see Figure 4(f)) and harmonic index (see Figure 4(g)), we obtain $TI(HDN3[n]) \leq TI(SHDN3[n])$.



(a) Comparison of $M_1(HDN3[n])$ with $M_1(SHDN3[n])$

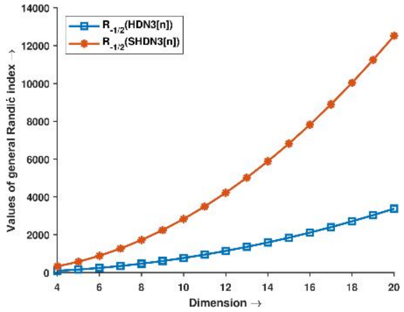


(b) Comparison of $M_2(HDN3[n])$ with $M_2(SHDN3[n])$

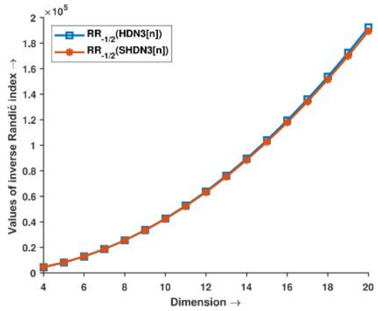


(c) Comparison of $mM_2(HDN3[n])$ with $mM_2(SHDN3[n])$

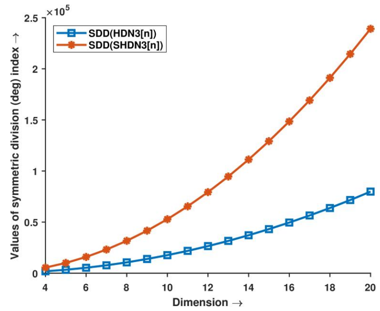
Remark 5. In Figure 4(e), the comparison plot of TI for $RR_{-1/2}(HDN3[n])$ and $RR_{-1/2}(SHDN3[n])$ seems to be overlapping due to the proximity of their numerical values for different dimensions. In fact, in the comparison plot of the inverse Randić index (for $\alpha = -1/2$) for the $HDN3[n]$ and $SHDN3[n]$ networks, we observed that



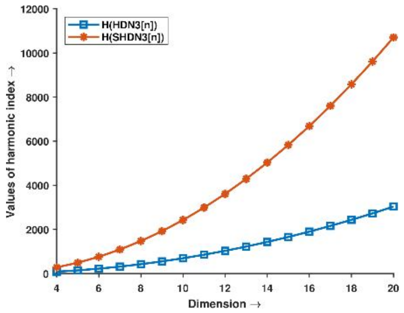
(d) Comparison of $R_{-1/2}(HDN3[n])$ with $R_{-1/2}(SHDN3[n])$



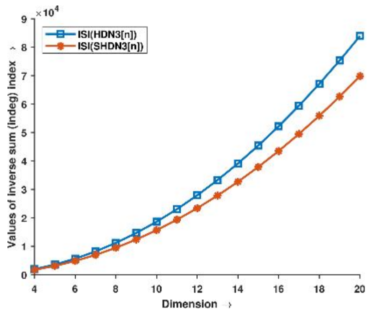
(e) Comparison of $RR_{-1/2}(HDN3[n])$ with $RR_{-1/2}(SHDN3[n])$



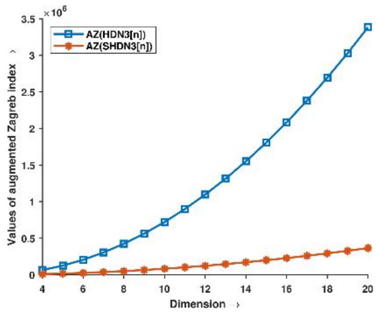
(f) Comparison of $SDD(HDN3[n])$ with $SDD(SHDN3[n])$



(g) Comparison of $H(HDN3[n])$ with $H(SHDN3[n])$



(h) Comparison of $ISI(HDN3[n])$ with $ISI(SHDN3[n])$



(i) Comparison of AZ$(HDN3[n])$ with $AZ(SHDN3[n])$

Figure 4. A comparative depiction of the degree-based topological indices of $HDN3[n]$ and $SHDN3[n]$ networks, where $4 \leq n \leq 20$

$RR_{-1/2}(HDN3[n]) \leq RR_{-1/2}(SHDN3[n])$ when we increased dimension $n = 4$ to 7 but for the dimension $n = 8$ to onwards, we see $RR_{-1/2}(HDN3[n]) \geq RR_{-1/2}(SHDN3[n])$.

III. Comparative Studies of $CHDN3[n]$ and $SCHDN3[n]$ Networks Based on Their M-Polynomials

This section comprises the comparative analysis between the degree-based topological characteristics of $CHDN3[n]$ and $SCHDN3[n]$ networks. The comparative evaluation of M-polynomials and associated topological indices for the $CHDN3[n]$ and $SCHDN3[n]$ networks has been carried out in Section F and requisites the findings are summarized in Section E.

E. Existing Results on $CHDN3[n]$ and $SCHDN3[n]$ Networks

The results that already exist for the M-polynomials and related degree-based topological indices of the $CHDN3[n]$ and $SCHDN3[n]$ networks are reported in this section. The expression of the M-polynomial of the $CHDN3[n]$ network is enclosed in Theorem 6, and their respective topological indices are mentioned in Theorem 7. Similarly, the expression of the M-polynomial of the $SCHDN3[n]$ network is comprised in Theorem 8, and their associated topological indices are outlined in Theorem 9.

Theorem 6 ([15])**.** *Let $CHDN3[n]$ signifies the third type of chain Hex-derived network of dimension n. Then a M-polynomial of the $CHDN3[n]$ network, where $n \geq 2$, is*

$$M(CHDN3[n]; x, y) = (5n + 6)x^4y^4 + (6n - 4)x^4y^8 + (n - 2)x^8y^8.$$

Theorem 7 ([15])**.** *Let $CHDN3[n]$ represents the third type of chain Hex-derived network of dimension n. Then*

(i) $M_1(CHDN3[n]) = 32(4n - 1)$,

(ii) $M_2(CHDN3[n]) = 336n - 160$,

(iii) $mM_2(CHDN3[n]) = \frac{33}{64}n + \frac{7}{32}$,

(iv) $R_\alpha(CHDN3[n]) = 4^{2\alpha}(5n + 6) + 32^\alpha(6n - 4) + 8^{2\alpha}(n - 2)$,

(v) $RR_{\alpha(CHDN3[n])} = \frac{1}{4^{2\alpha}}(5n+6) + \frac{1}{32^{\alpha}}(6n-4) + \frac{1}{8^{2\alpha}}(n-2)$,

(vi) $SDD(CHDN3[n]) = 27n - 2$,

(vii) $H(CHDN3[n]) = \frac{19}{8}n + \frac{7}{12}$,

(viii) $ISI(CHDN3[n]) = 30n - \frac{20}{3}$,

(ix) $AZ(CHDN3[n]) = \frac{1}{385875}(149316779n - 80401408)$.

Theorem 8 ([17]). *Let $SCHDN3[n]$ be the subdivided chain Hex-derived network of third type of dimension n. Then the expression of M-polynomial of the $SHDN3[n]$ network, where $n \geq 2$, is*

$$M(SCHDN3[n]; x, y) = (16n+8)x^2y^4 + (8n-8)x^2y^8.$$

Theorem 9 ([17]). *Let $SCHDN3[n]$ be the subdivided chain Hex-derived network of third type of dimension n. Then*

(i) $M_1(SCHDN3[n]) = 16(11n-2)$,

(ii) $M_2(SCHDN3[n]) = 64(4n-1)$,

(iii) $mM_2(SCHDN3[n]) = \frac{1}{2}(5n+1)$,

(iv) $R_\alpha(SCHDN3[n]) = 8^\alpha(16n+8) + 16^\alpha(8n-8)$,

(v) $RR_\alpha(SCHDN3[n]) = \frac{1}{8^\alpha}(16n+8) + \frac{1}{16^\alpha}(8n-8)$,

(vi) $SDD(SCHDN3[n]) = 2(37n-7)$,

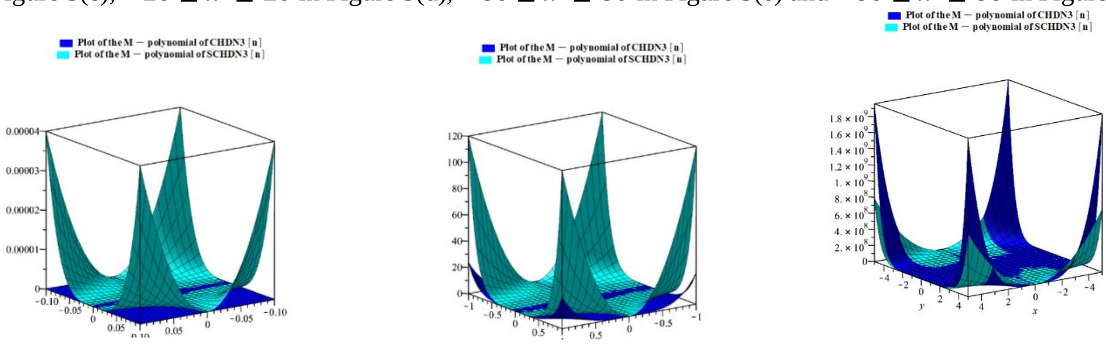
(vii) $H(SCHDN3[n]) = \frac{8}{15}(13n+2)$,

(viii) $ISI(SCHDN3[n]) = \frac{35}{15}(16n-1)$,

(ix) $AZ(SCHDN3[n]) = 192n$.

F. Main Results: Comparative Analysis Between the $CHDN3[n]$ and $SCHDN3[n]$ Networks

In this part, for the comparative study between the $CHDN3[n]$ and $SCHDN3[n]$ networks in the context of the M-polynomials and the associated topological indices of these networks, we use the above theorems. With the help of Maple 2020 software, we graphically compare (see Figure 5) the M-polynomial expressions of the $CHDN3[n]$ and $SCHDN3[n]$ networks for $n = 2$, in a single frame for various ranges of x and y. The considered domains of x and y are: $-0.1 \leq x \leq 0.1$ in Figure 5(a), $-1 \leq x \leq 1$ in Figure 5(b), $-5 \leq x \leq 5$ in Figure 5(c), $-10 \leq x \leq 10$ in Figure 5(d), $-30 \leq x \leq 30$ in Figure 5(e) and $-50 \leq x \leq 50$ in Figure 5(f).

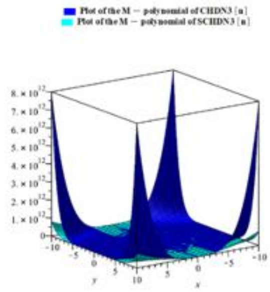


(a) M-polynomial comparison of $CHDN3[2]$ and $SCHDN3[2]$ networks, where $-0.1 \leq x, y \leq 0.1$.

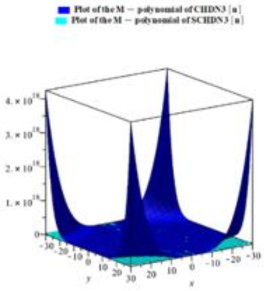
(b) M-polynomial comparison of $CHDN3[2]$ and $SCHDN3[2]$ networks, where $-1 \leq x, y \leq 1$.

(c) M-polynomial comparison of $CHDN3[2]$ and $SCHDN3[2]$ networks, where $-5 \leq x, y \leq 5$.

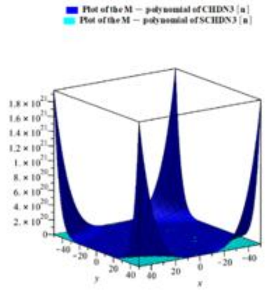
Moreover, comparison plots of the degree-based topological indices (*TI*) of the $CHDN3[n]$ and $SCHDN3[n]$ networks have been shown in Figure 6 using the MATLAB R2019a software. By examining Figure 6, we found $TI(CHDN3[n]) \leq TI(SCHDN3[n])$ for the first Zagreb index (see Figure 6(a)), modified second Zagreb index (see Figure 6(c)), general Randić index (see Figure 6(d) for $\alpha = -1/2$), inverse Randić index (see Figure 6(e) for $\alpha = -1/2$), symmetric division (deg) index (see Figure 6(f)), harmonic index (see Figure 6(g)), and inverse sum (indeg) index (see Figure 6(h)), while for the second Zagreb index (see Figure 6(b)) and augmented Zagreb index (see Figure 6(i)), we get $TI(CHDN3[n]) \geq TI(SCHDN3[n])$.



(d) M-polynomial comparison of $CHDN3[2]$ and $SCHDN3[2]$ networks, where $-10 \leq x, y \leq 10$

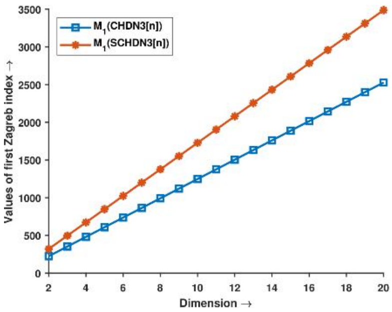


(e) M-polynomial comparison of $CHDN3[2]$ and $SCHDN3[2]$ networks, where $-30 \leq x, y \leq 30$

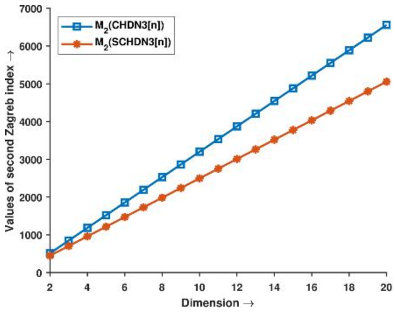


(f) M-polynomial comparison of $CHDN3[2]$ and $SCHDN3[2]$ networks, where $-50 \leq x, y \leq 50$

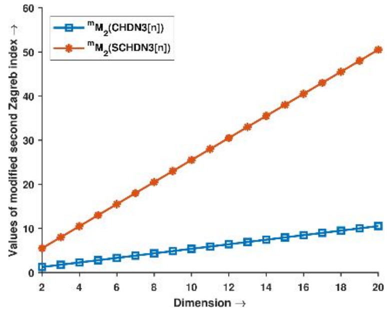
Figure 5. A comparative portrait of the M-polynomial of $CHDN3[2]$ and $SCHDN3[2]$ in different regions of x and y



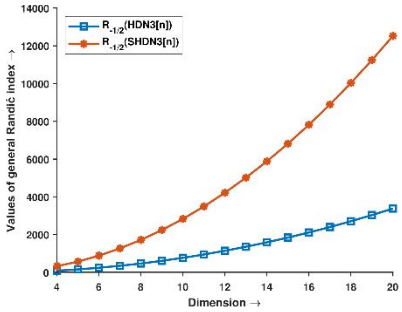
(a) Comparison of $M_1(CHDN3[n])$ with $M_1(SCHDN3[n])$



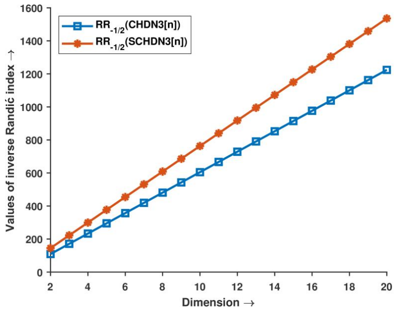
(b) Comparison of $M_2(CHDN3[n])$ with $M_2(SCHDN3[n])$



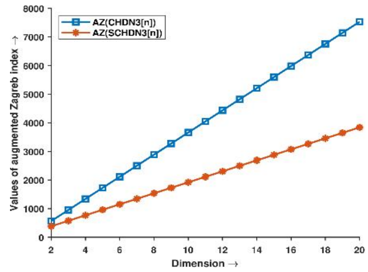
(c) Comparison of $mM_2(CHDN3[n])$ with $mM_2(SCHDN3[n])$



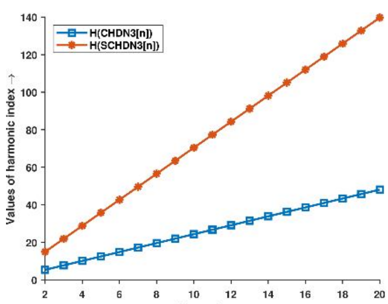
(d) Comparison of $R_{-1/2}(CHDN3[n])$ with $R_{-1/2}(SCHDN3[n])$



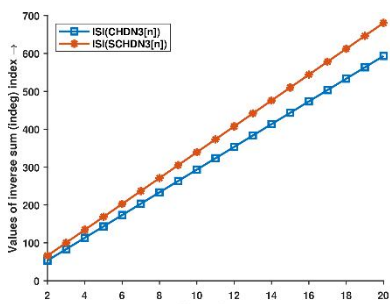
(e) Comparison of $RR_{-1/2}(CHDN3[n])$ with $RR_{-1/2}(SCHDN3[n])$



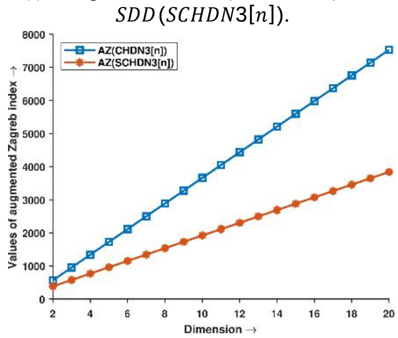
(f) Comparison of $SDD(CHDN3[n])$ with $SDD(SCHDN3[n])$.



(g) Comparison of $H(CHDN3[n])$ with $H(SCHDN3[n])$



(h) Comparison of $ISI(CHDN3[n])$ with $ISI(SCHDN3[n])$



(i) Comparison of $AZ(HDN3[n])$ with $AZ(SHDN3[n])$

Figure 6. A comparative depiction of the degree-based topological indices of $CHDN3[n]$ and $SCHDN3[n]$ networks, where $2 \leq n \leq 20$

IV. CONCLUSIONS

In this paper, we have considered two well-known Hex-derived networks of third type and their associated subdivisions. They are $HDN3[n]$, $CHDN3[n]$, and their subdivisions $SHDN3[n]$ and $SCHDN3[n]$, respectively. We performed a comparative analysis between the topological invariants of these Hex-derived networks. For the comparison purpose, we have portrayed the M-polynomials of each of the Hex-derived networks and their respective subdivisions in different regions of x and y. Furthermore, we have individually done comparative illustrations of the degree-based topological indices of these networks and their allied subdivisions. The outcomes discussed in this article may be helpful in demonstrating the relationship between the Hex-derived networks and their corresponding subdivisions.

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