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# MULTIPLE SQUARE SNAKE GRAPHS: THE M - POLYNOMIAL AND SOME DEGREE-BASED TOPOLOGICAL INDICES

*Alphy Jose*[1]
[1]*Assistant Professor, Little Flower College (Autonomous), Guruvayur, Kerala 680103, India*
**Emails:** *josealphy1012@gmail.com*[1]

## Abstract

*The computation of topological indices of graphs is a topic of current interest to many researchers since they are parameters which quantify the physio-chemical properties of the chemical graphs. The concept of M - polynomial of a graph G was introduced by Emeric Deutsch and Sandi Klavzar in 2015 as an effective tool to compute a closed formula for any such index for a given family of graphs. In this paper, the M - polynomial for the class of Multiple square snake graphs M_m (C_(4,n)) is calculated, which is then utilised to find the values of many degree based topological indices. Also, as additional results, the values of these topological indices for Square snake graphs, Double square snake graphs and Triple square snake graphs, which are special cases of the Multiple square snake graphs, are also enumerated. Topological indices are used as descriptors in QSPR/QSAR models and they help predict properties such as boiling point, stability, solubility, biological activity, toxicity, etc., without the need for experimental testing. Also, by means of these numbers, instead of handling large and complicated molecular structures, chemists can work with indices that summarize structural features. This makes mathematical modeling and comparison between molecules much easier.*

**Keywords:** *Degree-based Topological indices; M – polynomial; Multiple square snake graphs*

## 1. Introduction

Graph Theory is being extensively studied by researchers worldwide due to its applicability in real-life situations. In these, Chemical graph theory plays a vital role. A visual representation of a molecule is a graph in which vertices are atoms and edges are the chemical bonds between them. Many physio-chemical properties of these molecules can be easily understood by pure mathematical computation of parameters, called Topological indices. A graph is G(V,E) where V is the vertex set and E is the edge set, respectively. The order of the graph is $|V(G)| = n$ and the size of the graph is $|E(G)| = m$. Only simple, connected graphs are considered in this paper. The Degree of a vertex which is denoted by d(u), is the no. of vertices adjacent to a vertex u. A Topological index (TI) for a graph is

$$TI(G) = \sum_{uv\in E(G)} F(d(u), d(v))$$

where F is a proper function with the property that $F(x,y)= F(y,x)$.Topological indices are crucial for describing and characterizing the molecular structure. Chemist Harold Weiner introduced the first topological index in 1947, termed the Weiner index which is applied for the calculation of the boiling points of some alkane isomers [11]. In 1975, Randic [9] proposed the subsequent index called the Randic index which was designed to measure the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. It was demonstrated that the Randic index is well correlated with a variety of physio-chemical properties of alkanes, such as boiling point, enthalpy of formation, surface area, and solubility in water. After that numerous topological indices were introduced and studied for many graph classes and the studies are being continued to be relevant for its significance in real life scenario via Chemical applications. There are many methods to compute the values of topological indices. One among them is the use of M-polynomials which plays the role for degree-based invariants like Hosoya Polynomial for distance-based invariants. The concept of M - polynomial of a graph G was introduced by Emeric Deutsch and Sandi Klavzar [4] in 2015 as an effective tool to compute a closed formula for any such index for a given family of graphs. Let m_ij be the number of edges in G with end vertices of degrees i and j,δ ≤ i ≤ j ≤ Δ where δ and Δ are the minimum and maximum degrees of G, respectively, then the M - polynomial of G is defined as

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

**Table 1** **Some Topological indices using $M-$polynomial**

| Topological Index | Definition | Derivation from M(G;x,y) |
|---|---|---|
| First Zagreb Index $M_1$ | $\sum_{uv\in E(G)} d(u)+d(v)$ | $(D_x+D_y)(M(G;x,y)\|_{x=y=1}$ |
| Second Zagreb Index $M_2$ | $\sum_{uv\in E(G)} d(u).d(v)$ | $(D_x.D_y)(M(G;x,y)\|_{x=y=1}$ |
| Modified Second Zagreb Index ${}^mM_2$ | $\sum_{uv\in E(G)} \frac{1}{d(u).d(v)}$ | $(S_x.S_y)(M(G;x,y)\|_{x=y=1}$ |
| General Randic Index $R_\alpha$ | $\sum_{uv\in E(G)} (d(u)d(v))^\alpha$ | $(D_x^\alpha.D_y^\alpha)(M(G;x,y)\|_{x=y=1}$ |
| Harmonic Index $H$ | $\sum_{uv\in E(G)} \frac{2}{d(u)d(v)}$ | $2S_xJ(M(G;x,y)\|_{x=1}$ |
| Symmetric Division Index $SSD$ | $\sum_{uv\in E(G)} \left(\frac{d(u)}{d(v)}) + (\frac{d(v)}{d(u)}\right)$ | $(D_xS_y+S_xD_y)(M(G;x,y)\|_{x=y=1}$ |

where the operators D_x,D_y,S_x,S_Y and J are defined as

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

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

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

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

$$J(F(x,y)) \;=\; F(x,x)$$

Special graph class called as the Snake graphs are studied in different contexts in Mathematics in many diverse areas. They have finite or infinite, one or two dimensional repetitions of some geometric shape. The wide variety of applications of this structure can be found in [1], [2], [3], [5] and computations of some topological indices of different types of square snake graphs are found in [8], [6], [7], [10]. In this paper, the M - polynomial for the class of Multiple square snake graphs M_m (C_(4,n)) is found out, which is then utilised to find the values of many degree-based TI's. Also, as additional results, the values of these TI's for Square snake graphs, Double square snake graphs and Triple square snake graphs are also calculated. This paper gives a generalised method to find different topological indices of many important class of graphs which simplifies the process of finding them individually.

## 2. Topological Indices Of Multiple Square Snake Graphs

### 2.1. Multiple Square Snake Graphs

A multiple square snake graph M_m (C_(4,n)) is a graph obtained by replacing everyedge of a path P_(n+1)by m− multiple square graphs C_4, as shown in Fig.1.

Here $|V(M_m(C_{4,n})| = n(2m+1)+1$ and $|E(M_m(C_{4,n})| = 4\text{mn}$

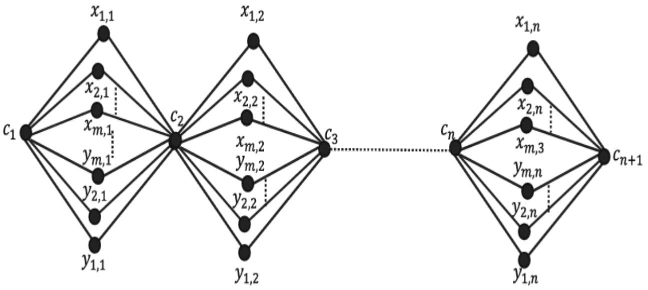

**Figure 1** **Multiple Square Snake Graph M_m (C_(4,n))**

The special cases of Multiple Square Snake Graphs are Square Snake Graphs when m = 1 as in Fig. 2, Double Square Snake Graphs when m = 2 as in Fig. 3 and Triple Square Snake Graphs when m = 3 as in Fig. 4.

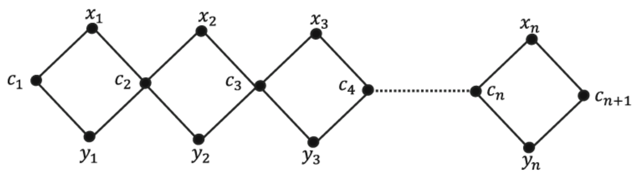

**Figure 2** **Square Snake Graph C_(4,n)**

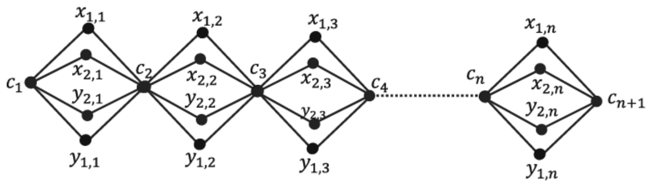

**Figure 3** **Double Square Snake Graph D(C_(4,n))**

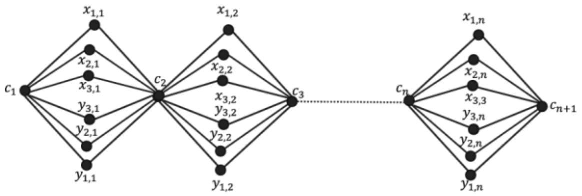

**Figure 4** **Triple Square Snake Graph T(C_(4,n))**

Now, the $M -$ Polynomial of $M_m(C_{4,n})$, by edge partitioning method, is calculated and used to enumerate the values of topological indices.

### Theorem 2.1:

The M- Polynomial of Multiple square snake graph $M_m$ (C_($_{4,n}$)) is given by
(M_m (C_($_{4,n}$) ); $_{x,y}$)= $4mx^2\ y^{2m}$+4m(n - 1)$x^2y^4$m

**Proof.**
The proof is based on the vertex partitions and edge partitions of M_m (C_(4,n) ).
The vertex degrees of M_m (C_(4,n) )are 2,2m and 4m with number of vertices as in the next table

| $d(u)$ | No. of Vertices |
|---|---|
| 2 | $2mn$ |
| $2m$ | 2 |
| $4m$ | $n-1$ |

Also, the edge partitions of M_m (C$_{4,n}$) is given by

$$E_1(M_m(C_{4,n}) = \{uv \in E(G); d(u) = 2m, d(v) = 2\}$$
$$E_2(M_m(C_{4,n}) = \{uv \in E(G); d(u) = 4m, d(v) = 2\}$$
with $|E_1(M_m(C_{4,n})| = 4m$ and
$|E_1(M_m(C_{4,n})| = 4m(n-1)$

Then, by the definition, the M- Polynomial is given by

$$M(M_m(C_{4,n});\ x,y) = \sum_{\le i \le j \le \Delta} m_{ij}\, x^i y^j$$
$$= m_{2,2m}x^2y^{2m} + m_{2,4m}x^2y^{4m}$$
$$= 4mx^2y^{2m} + 4m(n - 1)x^2y^{4m}$$

The next two results are used to calculate the values of TI's using M(G; x,y).

### Theorem 2.2 [4]:

Let $G$ be a graph and let
$TI(G) = \sum_{uv\in E(G)} F(d(u), d(v))$ where
$F(x,\ y) = \sum_{i,j\in Z} \alpha_{ij}\, x^i\, y^j$. Then
$TI(G) = F(D_x, D_y)(M(G; x, y))|x = y = 1$

### Theorem 2.3 [4]:

Let $G$ be a graph and let $TI(G) =$
$\sum_{uv\in E(G)} F(d(u), d(v))$ where $F(x, y) = \frac{x^r y^s}{(x+y+\alpha)^k}$
and $r, s \ge 0, t \ge 1$ and $\alpha \in Z$.Then
$TI(G) = (S_x{}^k Q_\alpha J D_x{}^r D_y{}^s)(M(G; x, y))|x = y = 1$

### Theorem 2.3 [4]:

Let $G$ be a graph and let $TI(G) =$
$\sum_{uv\in E(G)} F(d(u), d(v))$ where $F(x, y) = \frac{x^r y^s}{(x+y+\alpha)^k}$
and $r, s \ge 0, t \ge 1$ and $\alpha \in Z$.Then
$TI(G) = (S_x{}^k Q_\alpha J D_x{}^r D_y{}^s)(M(G; x, y))|x = y = 1$

### Theorem 2.4:

Let $G = M_m(C_{4,n})$ be the Multiple Square Snake graph. Then

1. $M_1(G) = 8m[n + m(2n - 1)]$
2. $M_2(G) = 16m^2(2n - 1)$
3. ${}^mM_2(G) = \frac{n+1}{2}$
4. $R_\alpha(G) = 2^{2\alpha+2}m^{\alpha+1}[4n - 3]$
5. $H(G) = \frac{4m(m+n+mn)}{(m+1)(2m+1)}$

6. $SSD(G) = 2(n+1)4m^2(2n-1)\$$

**Proof.**
By Theorem 2.1, M- Polynomial of Multiple square snake graph $M_m(C_{4,n})$ is given by

$$M\big(M_m(C_{4,n});\ x,y\big) = 4mx^2y^{2m} + 4m(n-1)x^2y^{4m}$$

Then,

1. $D_x(M(G;x,y) = 8mx^2y^{2m}[1+(n-1)y^{2m}]$

$D_y(M(G;x,y) = 8m^2x^2y^{2m}[1+2(n-1)y^{2m}]$

Hence,

$$M_1(G) = (D_x + D_y)(M(G;x,y)|_{x=y=1} = 8m[n+m(2n-1)]$$

2. $M_2(G) = (D_x.D_y)(M(G;x,y)|_{x=y=1}$

$= D_x(8m^2x^2y^{2m}[1+2(n-1)y^{2m}])|_{x=y=1}$

$= 16m^2(2n-1)$

1. $S_y\big(M(G;x,y)\big) = x^2y^{2m}[2+(n-1)y^{2m}]$

$$(S_x.S_y)(M(G;x,y) = \frac{x^3y^{2m}}{3}[2+(n-1)y^{2m}]$$

$${}^mM_2(G) = (S_x.S_y)(M(G;x,y)|_{x=y=1} = \frac{n+1}{3}$$

2. $D_y^\alpha\big(M(G;x,y)\big) = 2^{\alpha+1}m^{\alpha+1}x^2y^{2m} + 2^{\alpha+4}m^{\alpha+1}(n-1)x^2y^{4m}$

$$(D_x^\alpha.D_y^\alpha)(M(G;x,y)) = 2^{2\alpha+2}m^{\alpha+1}x^2y^{2m} + 2^{2\alpha+4}m^{\alpha+1}(n-1)x^2y^{4m}$$

$$R_\alpha(G) = 2^{2\alpha+2}m^{\alpha+1}(4n-3)$$

3. $J(M(G;x,y)) = 4mx^{2m+2} + 4m(n-1)x^{4m+2}$

$$S_xJ(M(G;x,y)) = \left(\frac{2mx^{2m+2}}{m+1}\right) + \left(\frac{2m(n-1)x^{4m+2}}{2m+1}\right)$$

$$H(G) = 2S_xJ(M(G;x,y)|_{x=y=1} = \frac{4m(m+n+mn)}{(m+1)(2m+1)}$$

4. $D_xS_y(M(G;x,y)) = 2x^2y^{2m}[2+(n-1)y^{2m}]$

$$S_xD_y(M(G;x,y)) = 4m^2y^{2m}[1+2(n-1)y^{2m}]$$

$$SSD(G) = (D_xS_y + S_xD_y)(M(G;x,y)|_{x=y=1} = 2(n+1)4m^2(2n-1)$$

## Theorem 2.5

The topological indices of Square snake graph $C_{4,n}$, Double square snake graph $D(C_{4,n})$ and Triple square snake graph $T\big(C_{4,n}\big)$ are given by

First Zagreb Index $M_1$:

$M_1(C_{4,n}) = 8(3n-1)$

$M_1(D(C_{4,n})) = 16(5n-2)$

$M_1(T(C_{4,n})) = 24(7n-3)$

Second Zagreb Index $M_2$:

$M_2(C_{4,n}) = 16(2n-1)$

$M_2(D(C_{4,n})) = 64(2n-1)$

$M_2(T(C_{4,n})) = 144(2n-1)$

Modified Second Zagreb Index ${}^mM_2$:

${}^mM_2(C_{4,n}) = \frac{n+1}{2}$

${}^mM_2(D(C_{4,n})) = \frac{n+1}{2}$

${}^mM_2T((C_{4,n})) = \frac{n+1}{2}$

General Randic Index $R_\alpha$:

$R_\alpha(C_{4,n}) = 2^{2\alpha+2}(4n-3)$

$R_\alpha\Big(D\big(C_{4,n}\big)\Big) = 2^{3(\alpha+1)}(4n-3)$

$R_\alpha(T(C_{4,n})) = 2^{(2\alpha+1)}3^{\alpha+1}(4n-3)$

Harmonic Index $H$:

$$H(C_{4,n}) = \frac{2(2n+1)}{3}$$

$$H(D(C_{4,n})) = \frac{8(3n+2)}{15}$$

$$H(T(C_{4,n})) = \frac{3(4n+3)}{7}$$

*Symmetric Division Index SSD*:

$$SSD(C_{4,n}) = 2(5n - 1)$$

$$SSD(D(C_{4,n})) = 2(17n - 7)$$

$$SSD(T(C_{4,n})) = 2(37n - 35)$$

## Conclusion

In this paper, various degree based Topological indices of Multiple Square snake graphs are calculated. These values are used to deduct the topological index values of the special graphs, like Square snake graphs, Double square snake graphs and multiple square snake graphs. These values of these complex graphs can be utilised to study many properties of chemical molecules with these underlying structures.

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