Research Article

Characterization of Extremal Unicyclic Graphs Using F -Coindex

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The study of forgotten index and coindex for the molecular structures of some special chemical graphs (compounds and drugs) has proven significant in medical and pharmaceutical drug design fields by making reliable statistical conclusion about biological properties of new chemical compounds and drugs. In mathematical chemistry, finding extreme graphs with respect to topological index is an active area of research. The aim of this paper is to characterize the family of unicyclic graphs with extreme (largest and smallest) F -coindex. Moreover, the study also contains different other properties of unicyclic graphs. All these results are based upon an alternative form of F -coindex which is established with the help of special property in the graphs.

1. Introduction

There is a continuous rise in various new diseases every year, the reason being different novel viruses and bacteria. In order to overcome such diseases, introduction of high-quality drugs is of prime significance. Importance of topological indices is a well-established fact for nanotechnology in isomer discrimination, pharmaceutical drug design, structure-property relationship, and structure-activity relationship (for details, see [1–3]). In 1972, Gutman and Trinajstić [4] approximated formulas for the total π -electron energy (E). Among the formulas presented in [4], a pair of topological indices was studied more frequently than any other indices. These pairs of indices are known as Zagreb first and second indices denoted by symbols M_1 and M_2 , respectively. A detailed study of these indices can be found in [5]. Other than M_1 and M_2 , another formula depending upon sum of cubes of vertex degrees was also presented in [4]. In order to shed some light on this important index, Furtula and Gutman [6] established some of its basic properties of F -index (“forgotten topological index”). Furtula and Gutman [6] further showed that F -index can improve physicochemical applicability of M_1 ,

significantly. Also, by assuming the linear model, they enhanced the predictive ability of these indices. While working on weighted Wiener polynomial of graphs, Doslic [7] initiated work on coindices by introducing Zagreb coindices. Formal definitions of Zagreb coindices and basic properties were reported by Ashrafi et al. [8]. De et al. [9] studied some key features of F -coindex. In [9], the authors compared the correlation of the logarithm of the octanol-water partition coefficient (P) with F -coindex, M_1 , and F . They came out with result that correlation coefficient between $\log P$ and F -coindex is stronger than that of M_1 and F . They concluded that F -coindex can predict the $\log P$ values with high accuracy. The study of F -index and F -coindex is an active area of research nowadays, and we can find a number of results, for example, [10–14]. Recently, Amin et al. [15] studied about minimal trees using F -coindex. The results in [15] are only about first, second, and third minimum trees. Very recently, Akther et al. [16] deduced the results for extremal graphs for F -index among the classes of connected unicyclic and bicyclic graphs. In the present work, we provide an alternative form of F -coindex to study different properties of unicyclic graphs. Moreover, these properties are further used to study extremal graphs for F -coindex for the family of unicyclic graphs.

Throughout the work we assume that $G(V(G), E(G))$ be a graph where $V(G)$ and $E(G)$, respectively, denote vertex and edge sets. Also, $G(V(G), E(G))$ is a connected graph with order $|V(G)|$ and size $|E(G)|$. An adjacent edge is denoted by $e = uv \in E(G)$, whereas $uw \notin E(G)$ is used to denote that u and w are not adjacent. For any $u \in V(G)$ (or $u \in G$), d_u represents the degree of u . Here we use N_u to denote the number of vertices not adjacent to $u \in G$; mathematically,

$$N_u = |\{\omega \mid u\omega \notin E(G)\}|, \quad \text{for each } u \in G. \quad (1)$$

Forgotten topological index is defined by Gutman and Trinajstić [4].

$$F(G) = \sum_{v \in V(G)} d_v^3. \quad (2)$$

Equation (2) can be written as [4]

$$F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2). \quad (3)$$

Hu et Al. [17] proposed a general form of zeroth-order Randić index given as follows:

$${}^0R_\alpha(G) = \sum_{u \in G} d_u^\alpha = \sum_{uv \in E(G)} (d_u^{\alpha-1} + d_v^{\alpha-1}), \quad (4)$$

α is an arbitrary real number.

It can be noted that forgotten index can be obtained for $\alpha = 3$. Similarly, Mansour and Song [18] introduced a general formula for zeroth-order Randić coindex as given below:

$$\overline{{}^0R_\alpha}(G) = \sum_{uv \notin E(G)} (d_u^{\alpha-1} + d_v^{\alpha-1}). \quad (5)$$

For $\alpha = 3$, the above formula takes the form of F-coindex used by De et al. [9].

$$\overline{F}(G) = \sum_{uv \notin E(G)} (d_u^2 + d_v^2). \quad (6)$$

Very recently, Milovanović et al. [19] proved the following formula for zeroth-order Randić coindex:

$$\overline{{}^0R_\alpha}(G) = \sum_{u \in (G)} (n-1-d_u) d_u^{\alpha-1}, \quad (7)$$

for all real values of α . Working independently, Ali et al. [20] published the following forms of F-coindex given by equation (6):

$$\overline{F}(G) = \sum_{u \in G} d_u^2 \times N_u. \quad (8)$$

Also,

$$\overline{F}(G) = \sum_{u \in G} [(n-1)d_u^2 - d_u^3], \quad (9)$$

where the number of nonadjacent vertices to u is given by

$$N_u = n-1-d_u. \quad (10)$$

The F-coindex is also called Lanzhou Index. In 2021, Dehgard and Liu [21] characterized trees with fixed

maximum degree using the Lanzhou Index. We can easily calculate F-coindex, using formula given by equation (8), for some well-known graphs. Let P_n , C_n , $K_{1,n-1}$, and K_n be the path, cycle, star, and complete graphs on n vertices. Then, F-coindex for these graphs is as follows:

- (1) $\overline{F}(P_n) = 4n^2 - 18n + 20$.
- (2) $\overline{F}(C_n) = 4n^2 - 12n$.
- (3) $\overline{F}(K_{1,n-1}) = (n-1)(n-2)$.
- (4) $\overline{F}(K_n) = 0$ and $\overline{F}(\overline{K_n}) = 0$.

Note here that we reserve $\overline{F}_{u_i}$ to represent contribution of i vertices towards F-coindex of graph $\overline{F}(G)$.

2. F-Coindex of Unicyclic Graphs

Unicyclic graphs are connected graphs with equal number of vertices and edges. Let U_n denote the set of the unicyclic graphs with n vertices and U_n^k denote the class of all unicyclic graphs with n vertices having a cycle of length k . Let $U_n^k(p_1, p_2, \dots, p_k) \in U_n^k$ denote a unicyclic graph with n vertices having cycle of length k , and each vertex i of cycle has p_i pendant vertices on it, where $1 \leq i \leq k$.

For example, $U_{14}^3(5, 4, 2)$, shown in Figure 1, represents a unicyclic graph with 14 vertices having a cycle of length 3, where these 3 vertices of cycle have 5, 4, and 2 pendants, respectively. It is important to note that in $U_n^k(p_1, p_2, \dots, p_k)$, $k + p_1 + p_2 + \dots + p_k = n$.

Theorem 1. Let $G \in U_n$ and d_u be the degree of vertex $u \in V(G)$. Let $u^* \in V(G)$ be the vertex with maximum contribution towards $\overline{F}(G)$; then, degree of the vertex u^* is given by

$$d_{u^*}^* = \begin{cases} \left\lfloor \frac{2}{3}(n-1) \right\rfloor, & \text{if } n \equiv 2 \pmod{3}, \\ \left\lfloor \frac{2}{3}(n-1) \right\rfloor, & \text{otherwise.} \end{cases} \quad (11)$$

Proof. From equation (9), we know that F-coindex of a graph is given by

$$\overline{F}(G) = \sum_{u \in G} [(n-1)d_u^2 - d_u^3]. \quad (12)$$

Let u^* with degree d_{u^*} have maximum contribution towards $\overline{F}$; then,

$$\frac{\partial \overline{F}}{\partial d_{u^*}} = 2(n-1)d_{u^*} - 3(d_{u^*})^2 = 0, \quad \text{this gives } d_{u^*} = \frac{2(n-1)}{3}. \quad (13)$$

Also, note that

$$\frac{\partial^2 \overline{F}}{\partial d_{u^*}^2} = -2(n-1) < 0. \quad (14)$$

This implies that the vertex with degree $d_{u^*} = (2(n-1)/3)$ will have maximum contribution towards $\overline{F}(G)$. Note

FIGURE 1: For $U_{16}^3(5, 4, 2)$. FIGURE 2: For $U_n^3(n-3, 0, 0)$.

that d_{u^*} must be an integer value. To make d_{u^*} an integer value, we round off $d_{u^*} = (2(n-1)/3)$ to nearest integer value to get

$$d_{u^*} = \begin{cases} \left\lceil \frac{2}{3}(n-1) \right\rceil, & \text{if } n \equiv 2 \pmod{3}, \\ \left\lfloor \frac{2}{3}(n-1) \right\rfloor, & \text{otherwise.} \end{cases} \quad (15)$$

□

According to Theorem 1, it is evident that contribution of a vertex towards F -coindex in a unicyclic graph increases with an increase in degree of the vertex until degree of the vertex reaches a value given by equation (11).

Theorem 2. For $n \geq 4$, $U_n^3(n-3, 0, 0)$ has minimum F -coindex among the family of unicyclic graphs. The F -coindex for $U_n^3(n-3, 0, 0)$ is given by

$$\overline{F}(U_n^3(n-3, 0, 0)) = (n-3)(n+6). \quad (16)$$

Proof. First, we will calculate $\overline{F}(U_n^3(n-3, 0, 0))$ and then show that it is minimum F -coindex among the family of unicyclic graphs.

It is obvious from the structure of $U_n^3(n-3, 0, 0)$ that there would be a cycle of length 3 and all pendant vertices will be there on a single vertex of the cycle and there would be two vertices of degree 2, as shown in Figure 2. From Figure 2, it is clear that one vertex of the cycle has degree $n-1$ having $n-3$ pendants. The details of $U_n^3(n-3, 0, 0)$ are given in Table 1.

Using the formula given by equation (8) and information given in Table 1, we get

$$\begin{aligned} \overline{F}(U_n^3(n-3, 0, 0)) &= (n-3) \left[(1)^2 \cdot (n-2) \right] + 2 \left[(2)^2 \cdot (n-3) \right] \\ &= (n-3)(n-2) + 8(n-3) = (n-3)(n+6). \end{aligned} \quad (17)$$

$$\text{Thus, } \overline{F}(U_n^3(n-3, 0, 0)) = (n-3)(n+6).$$

TABLE 1: For $U_n^3(n-3, 0, 0)$.

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	2
$n-1$	0	1

Now we will show that $\overline{F}(U_n^3(n-3, 0, 0)) = (n-3)(n+6)$ is the minimum value of F -coindex for the family of unicyclic graph. From equations (8) and (9), contribution towards F -coindex of unicyclic graph increases with increase in degree of the vertex until

$$d_{u^*} = \begin{cases} \left\lceil \frac{2}{3}(n-1) \right\rceil, & \text{if } n \equiv 2 \pmod{3}, \\ \left\lfloor \frac{2}{3}(n-1) \right\rfloor, & \text{otherwise,} \end{cases} \quad (18)$$

as given in Theorem 1. We can note from Theorem 1 and equation (9) that the F -coindex can be minimized by minimizing each of the term that is contributing for each of the vertices. This can be further categorized as the following two facts.

Fact#1 More pendants and two-degree vertices will yield minimum F -coindex.

Fact#2 Vertex with degree $n-1$ will have zero contribution towards F -coindex of unicyclic graph.

It is also known that total degree of a graph is $2n$. If one of the vertices has degree $n-1$ with zero contribution towards F -coindex of unicyclic graph, then remaining $n-1$ vertices will have total degree $n+1$. Thus, instead of total degree $2n$, we are left with the degree $n+1$ that is contributing towards F -coindex of unicyclic graph in the form of pendants and two-degree vertices. The only possible structure for such a unicyclic graph is $n-3$ pendants and two vertices of two-degree, that is, $U_n^3(n-3, 0, 0)$. It is likewise established that in any other structure of unicyclic graph, there would be more vertices with higher degrees, ultimately contributing more towards F -coindex of unicyclic graph than $U_n^3(n-3, 0, 0)$. □

Theorem 3. Let $U_n^3(p_1, p_2, 0) \in U_n$ with p_1, p_2 be the pendants on u_1 and u_2 , respectively. If $|p_1 - p_2| \leq 1$, then the contribution of u_1 and u_2 towards $\bar{F}(G)$ is given by

$$\bar{F}_{u_i} = \begin{cases} \frac{1}{4}(n+1)^2(n-3), & \text{if } n \text{ is odd,} \\ \frac{1}{4}(n^3 - n^2 - 6n - 8), & \text{if } n \text{ is even,} \end{cases} \quad \text{for } i = 1, 2. \quad (19)$$

Also, $\bar{F}_{u_i}$, for $i = 1, 2$, is maximum when $|p_1 - p_2| \leq 1$.

Proof. Let $U_n^3(p_1, p_2, 0) \in U_n$ and n be an odd number and let $p_1 = p_2 = ((n-3)/2)$ be the pendants on u_1 and u_2 , respectively. In this case, both u_1 and u_2 will have degree $(1/2)(n+1)$ and both will be nonadjacent to $(1/2)(n-3)$. Thus, contribution of both of u_1 and u_2 towards F -coindex is given by

$$\bar{F}_{u_i} = 2 \cdot \left(\frac{1}{2}(n+1)\right)^2 \left(\frac{n-3}{2}\right) = \frac{1}{4}(n+1)^2(n-3), \quad (20)$$

for $i = 1, 2$.

Now let us assume that $U_n^3(p_1, p_2, 0) \in U_n$ and let n be an even number. Here u_1 and u_2 have $p_1 = (1/2)(n-2)$ and

$p_2 = (1/2)(n-4)$, respectively. In this case, $N_{u_1} = ((n-4)/2)$ and $N_{u_2} = ((n-2)/2)$. Thus, we obtain $\bar{F}_{u_i} = (1/4)(n^3 - n^2 - 6n - 8)$, for $i = 1, 2$.

Now we prove $\bar{F}_{u_i}$, for $i = 1, 2$, is maximum when $|p_1 - p_2| \leq 1$. On the contrary, assume that, for $|p_1 - p_2| > 1$, contribution of u^* and u^{**} towards $\bar{F}(G)$ is more than $\bar{F}_{u_i}$ for $i = 1, 2$. This means that there exists a positive integer $m \geq 1$ such that pendant at vertex u^* is $p_1 = ((n-3)/2) + m$ and similarly for u^{**} , $p_2 = ((n-3)/2) - m$ and

$$\bar{F}_{u^*, u^{**}} > \bar{F}_{u_i}, \quad \text{for } i = 1, 2. \quad (21)$$

Initially, we assume that n is odd. It is easy to see that

$$d_{u^*} = \frac{n+1}{2} + m, \quad (22)$$

$$d_{u^{**}} = \frac{n+1}{2} - m.$$

Note that

$$N_{u^*} = \frac{n+1}{2} - m, \quad (23)$$

$$N_{u^{**}} = \frac{n+1}{2} + m.$$

Thus,

$$\begin{aligned} \bar{F}_{u^*, u^{**}} &= \left(\frac{n+1}{2} + m\right)^2 \left(\frac{n+1}{2} - m\right) + \left(\frac{n+1}{2} - m\right)^2 \left(\frac{n+1}{2} + m\right) \\ &= \frac{1}{4}(n+1)^2(n-3) - [nm^2 + n^2m + nm + 5m^2] \\ &< \frac{1}{4}(n+1)^2(n-3), \quad \text{since } m, n \geq 1. \end{aligned} \quad (24)$$

Now assume that n is even; then, we have

$$\begin{aligned} d_{u^*} &= \frac{n+2}{2} + m, \\ d_{u^{**}} &= \frac{n}{2} - m. \end{aligned} \quad (25)$$

Note that

$$\begin{aligned} N_{u^*} &= \frac{n-4}{2} - m, \\ N_{u^{**}} &= \frac{n-2}{2} + m, \end{aligned} \quad (26)$$

which gives

$$\begin{aligned} \bar{F}_{u^*, u^{**}} &= \left(\frac{n+2}{2} + m\right)^2 \left(\frac{n-4}{2} - m\right) + \left(\frac{n}{2} - m\right)^2 \left(\frac{n+2}{2} + m\right) \\ &= \frac{1}{4}(n^3 - n^2 - 6n - 8) - [m(m+1)(n+5)] \\ &< \frac{1}{4}(n^3 - n^2 - 6n - 8), \quad \text{since } m, n \geq 1. \end{aligned} \quad (27)$$

It is obvious that our assumption that equation (21) holds is wrong. Therefore, $\bar{F}_{u_i}$, for $i = 1, 2$, is maximum when $|p_1 - p_2| \leq 1$. $\square$

It is important to note here that if one vertex has degree d_{u^*} given by (11), then maximum possible degree of any

other vertex, say u^{**} , in a unicyclic graph would be $n - 3 - d_{u^{**}}$. Theorem 3 says that the contribution of both u^* and u^{**} towards $\overline{F}(G)$ would be less than that if both vertices having degrees states in Theorem 3.

Theorem 4. Let $U_n^k(p_1, p_2, \dots, p_k) \in U_n^k$ such that $|p_i - p_j| \leq 1$, for $1 \leq i, j \leq k$; then, $k = (2n/(n-4))$ maximizes F -coindex of unicyclic graph.

$$\begin{aligned} \overline{F}(U_n^k(p_1, p_2, \dots, p_k)) &= k \left[\frac{n-k}{k} + 2 \right]^2 \left[\frac{n(k-1) - 2k}{k} \right] + [(1)^2(n-k)(n-2)] \\ &= \frac{1}{k^2} [k^3(n-2) + k^2(2n^2 - 5n) + k(n^3 - 4n^2) - n^3] \\ &\quad + n^2 - kn - 2n + 2k \\ &= \frac{1}{k} (n^3 - 4n^2) - \frac{n^3}{k^2} + (3n^2 - 7n). \end{aligned} \quad (28)$$

In order to get the value of that maximizes $\overline{F}(U_n^k(p_1, p_2, \dots, p_k))$, we proceed as follows.

$$\frac{d\overline{F}}{dk} = 0, \quad \text{implies that } k = \frac{2n}{n-4}, \quad (29)$$

Also, note that for $k = (2n/(n-4))$, we have $(d^2\overline{F}/dk^2) < 0$. This means that $k = (2n/(n-4))$ maximizes $\overline{F}(U_n^k(p_1, p_2, \dots, p_k))$. $\square$

We know that k must be a positive integer. From the expression $k = (2n/(n-4))$, it can be seen that for large values of n , k approaches 2 but for values of n close to 11, k is closer to 3.

Theorem 5. For $n \geq 28$, let $U_n^3(p_1, p_2, 0) \in U_n^k$ with $p_1, p_2 \in \{\lfloor (n-3)/2 \rfloor, \lceil (n-3)/2 \rceil\}$, such that $p_1 + p_2 = n-3$. In this case,

$$\overline{F}(U_n^3(p_1, p_2, 0)) = \begin{cases} \frac{1}{4}(n-3)(n^2 + 6n + 9), & \text{if } n \text{ is odd,} \\ \frac{1}{4}(n^3 + 3n^2 - 10n - 32), & \text{if } n \text{ is even.} \end{cases} \quad (30)$$

Furthermore, values given by equation (30) are maximum F -coindex for the family of unicyclic graphs with $n \geq 28$.

Proof. Let $U_n^3(p_1, p_2, 0) \in U_n^k$, with $p_1, p_2 \in \mathbb{N}$ such that $p_1 + p_2 = n-3$ and

$$|p_1 - p_2| = \begin{cases} 1, & \text{if } n \text{ is even,} \\ 0, & \text{if } n \text{ is odd,} \end{cases} \quad \text{for } n \geq 28 \quad (31)$$

The structure of such graphs is shown in Figure 4.

Proof. Without loss of generality, we assume n such that each vertex has equal vertices, that is, $(1/k)(n-k)$. From Figure 3, we can have the following table.

It is obvious from the structure of $U_n^k(p_1, p_2, \dots, p_k)$ that there would be $(n-k)$ vertices of degree 1 and k vertices of degree $(1/k)(n+k)$ as shown in Figure 3.

Using the formula given by equation (8) and data given in Table 2, we get

From Figure 4, Tables 3 and 4 are tabulated. In this case, F -coindex is obtained by adding to $(n-3)(n+2)$ the contribution of pendants and degree 2 vertices in equation (19), respectively for odd and even values of n . Thus using the table given above, we may write

$$\overline{F}(U_n^3(p_1, p_2, 0)) = \begin{cases} \frac{1}{4}(n-3)(n^2 + 6n + 9), & \text{if } n \text{ is odd,} \\ \frac{1}{4}(n^3 + 3n^2 - 10n - 32), & \text{if } n \text{ is even.} \end{cases} \quad (32)$$

It can easily be verified that $\overline{F}(U_n^3(p_1, p_2, 0))$ given by equation (32) is maximum by using Theorems 3 and 4. $\square$

Theorem 6. For $11 \leq n \leq 27$, let $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $p_i \in \{\lfloor (n-3)/3 \rfloor, \lceil (n-3)/3 \rceil\}$, for $i = 1, 2, 3$, such that $\sum_{i=1}^3 p_i = n-3$; then,

$$\overline{F}(U_n^3(p_1, p_2, p_3)) = \begin{cases} \frac{2n^3}{9} + \frac{5n^2}{3} - 7n, & \text{if } n \equiv 0 \pmod{3}, \\ \frac{6n^3}{27} + \frac{5n^2}{3} - \frac{53n}{9} - 4, & \text{if } n \equiv 1 \pmod{3}, \\ \frac{2n^3}{9} + \frac{53n^2}{27} - 7n - \frac{22}{9}, & \text{if } n \equiv 2 \pmod{3}. \end{cases} \quad (33)$$

Proof. For $11 \leq n \leq 27$, let $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $p_1, p_2, p_3 \in \mathbb{N}$ such that $p_1 + p_2 + p_3 = n-3$; then, we have following three possible cases for p_1, p_2 , and p_3 .

Case I: when $n \equiv 0 \pmod{3}$, then $p_1 = p_2 = p_3 = ((n-3)/3)$.

TABLE 2: For $U_n^k(p_1, p_2, \dots, p_k)$ with $p_i = (1/k)(n-k)$, for $1 \leq i \leq k$.

d_u	N_u	Frequency
1	$n-2$	$n-k$
$((n-k)/k) + 2$	$((n(k-1) - 2k)/k)$	k

FIGURE 3: For $U_n^k(p_1, p_2, \dots, p_k)$ with $p_i = (1/k)(n-k)$, for $1 \leq i \leq k$.

Case II: when $n \equiv 1 \pmod{3}$, then $p_1 = \lceil (n-3)/3 \rceil$ and $p_2 = p_3 = \lfloor (n-3)/3 \rfloor$.

Case III: when $n \equiv 2 \pmod{3}$, then $p_1 = p_2 = \lceil (n-3)/3 \rceil$ and $p_3 = \lfloor (n-3)/3 \rfloor$.

Now we consider each case separately, to find the F-coindex of $U_n^3(p_1, p_2, p_3)$ for $11 \leq n \leq 27$.

Case I: when $n \equiv 0 \pmod{3}$, then $p_1 = p_2 = p_3 = ((n-3)/3)$, as shown in Figure 5(a). In this class, we discuss all graphs for $11 \leq n \leq 27$ when n is divisible by 3, that is, $n = 3k$, for $k = 4, 5, \dots, 9$. For such graphs, degree of each vertex of cycle is given by $((n+3)/3)$ and there are $(n-3)$ pendant vertices. From the figure, we have the following table.

Using the formula given by equation (8) and Table 5, we get

$$\overline{F}(G) = 3 \cdot \left(\frac{n+3}{3}\right)^2 \left(\frac{2}{3}(n-3)\right) + (n-2)(n-3). \quad (34)$$

Simplification of the above equation gives

$$\overline{F}(G) = \frac{2n^3}{9} + \frac{5n^2}{3} - 7n. \quad (35)$$

Case II: when $n \equiv 1 \pmod{3}$, then $p_1 = ((n-1)/3)$ and $p_2 = p_3 = ((n-4)/3)$, for $n = 3k+1$ where $k = 4, 5, \dots, 8$, as shown in Figure 5(b).

In this case, we have the following values of degrees, nonadjacent vertices, and frequencies.

Using the formula given by equation (8) and Table 6, we get

$$\begin{aligned} \overline{F}(G) &= 2\left(\frac{n+2}{3}\right)^2 \left(\frac{2n-5}{3}\right) + \left(\frac{n+5}{3}\right)^2 \left(\frac{2n-8}{3}\right) \\ &\quad + (n-3)(n-2). \end{aligned} \quad (36)$$

After simplifying last equation, we obtain

$$\overline{F}(G) = \frac{6n^3}{27} + \frac{5n^2}{3} - \frac{53n}{9} - 4. \quad (37)$$

Case III: in the last case, we consider the family of unicyclic graphs $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $n \equiv 2 \pmod{3}$. Here $p_1 = p_2 = ((n-2)/3)$ and $p_3 = ((n-5)/3)$ where $n = 3k+2$ for $k = 4, 5, \dots, 8$ (Figure 5(c)). It is easy to construct the following table.

Using the formula given by equation (8) and Table 7, we get

$$\begin{aligned} \overline{F}(G) &= 2\left(\frac{n+4}{3}\right)^2 \left(\frac{2n-7}{3}\right) + \left(\frac{n+1}{3}\right)^2 \left(\frac{2n-4}{3}\right) \\ &\quad + (n-3)(n-2). \end{aligned} \quad (38)$$

Thus, we obtain

$$\overline{F}(G) = \frac{2n^3}{9} + \frac{53n^2}{27} - 7n - \frac{22}{9}. \quad (39)$$

□

Theorem 7. Let $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $p_i \in \{\lfloor (n-3)/3 \rfloor, \lceil (n-3)/3 \rceil\}$, for $i = 1, 2, 3$, such that $p_1 + p_2 + p_3 = n-3$; then, $\overline{F}(U_n^3(p_1, p_2, p_3))$ has maximum F-coindex for the family of unicyclic graphs with $11 \leq n \leq 27$.

Proof. By Theorem 4, we know that $k = (2n/(n-4))$ maximizes F-coindex of unicyclic graph. This value must be integer as it represents number of vertices on which we should divide pendant vertices. The value of k given in Theorem 4 is close to 3 when $n = 11$ and it decreases as we increase n . Therefore, we can compare F-coindex of both values of k , that is, $k = 2$ and $k = 3$.

Without loss of generality, we assume that $n-3$ is even and divisible by 3, and it is equivalent to saying that n is odd and divisible by 3. It is evident from Figure 6 and Tables 8 and 9 that both $U_n^3(p_1, p_2, p_3)$ and $U_n^3(p_1, p_2, 0)$ have same pendant vertices with same number of nonadjacent vertices.

Therefore, contribution of pendant vertices would be same in both cases. It means that we should compare the contribution of other vertices for F-coindex of $U_n^3(p_1, p_2, p_3)$ and $U_n^3(p_1, p_2, 0)$. We can see that in $U_n^3(p_1, p_2, p_3)$, there are 3 vertices, say u_1, u_2 , and u_3 , with degree $((n+3)/3)$ with nonadjacent vertices $((2(n-3))/3)$.

$$\overline{F}_{u_i} = \frac{2}{9}(n+3)^2(n-3), \quad \text{for } i = 1, 2, 3, \quad (40)$$

FIGURE 4: $U_n^3(p_1, p_2, 0)$, $n \geq 28$. (a) n is odd. (b) n is even.TABLE 3: For $U_n^3((n-3)/2, (n-3)/2, 0)$.

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	1
$(1/2)(n+1)$	$(1/2)(n-3)$	2

TABLE 4: For $U_n^3((n-2)/2, (n-4)/2, 0)$.

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	1
$(n/2)$	$(1/2)(n-2)$	1
$(1/2)(n+2)$	$(1/2)(n-4)$	1

FIGURE 4: $U_n^3(p_1, p_2, p_3)$ with $p_i \in \{ \lfloor (n-3)/3 \rfloor, \lceil (n-3)/3 \rceil \}$, for $i = 1, 2, 3$.TABLE 5: For $U_n^3(p_1, p_2, p_3)$.

d_u	N_u	Frequency
$((n+3)/3)$	$(2/3)(n-3)$	3
1	$n-2$	$n-3$

TABLE 6: For $U_n^3(p_1, p_2, p_3)$.

d_u	N_u	Frequency
$(1/3)(n+2)$	$(1/3)(2n-5)$	2
$(1/3)(n+5)$	$(2/3)(n-4)$	1
1	$n-2$	$n-3$

TABLE 7: For $U_n^3(p_1, p_2, p_3)$.

d_u	N_u	Frequency
$(1/3)(n+4)$	$(1/3)(2n-7)$	2
$(1/3)(n+1)$	$(2/3)(n-2)$	1
1	$n-2$	$n-3$

FIGURE 4: $U_n^3(p_1, p_2, p_3)$ and $U_n^3(p_1, p_2, 0)$.TABLE 8: For $U_n^3(((n-3)/3), t((n-3)/3)n, q((n-3)/3))$.

d_u	N_u	Frequency
$((n+3)/3)$	$(2/3)(n-3)$	3
1	$n-2$	$n-3$

TABLE 9: For $U_n^3(((n-3)/2), ((n-3)/2), 0)$.

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	1
$((n+1)/2)$	$((n-3)/2)$	2

where $\bar{F}_{u_i}$, for $i = 1, 2, 3$, represents contribution of u_1, u_2 , and u_3 towards $\bar{F}(U_n^3(((n-3)/3), ((n-3)/3), ((n-3)/3)))$.

Similarly, for $U_n^3(p_1, p_2, 0)$, contribution of v_1, v_2 , and v_3 is given by

$$\bar{F}_{v_i} = \frac{1}{4}(n-3)(n^2 + 2n + 17), \quad \text{for } i = 1, 2, 3, \quad (41)$$

where $\bar{F}_{v_i}$, for $i = 1, 2, 3$, represents contribution of v_1, v_2 , and v_3 towards $\bar{F}(U_n^3(((n-3)/2), ((n-3)/2), 0))$. By analyzing equations (40) and (41), we have

$$\bar{F}_{u_i} = \bar{F}_{v_i}, \quad \text{for } n = 27, \text{ and } \bar{F}_{u_i} > \bar{F}_{v_i} \text{ for } 11 \leq n < 27. \quad (42)$$

In general, we can write

$$\begin{cases} \bar{F}(U_n^3(p_1, p_2, p_3)) > \bar{F}(U_n^3(p_1, p_2, 0)), & \text{for } 11 \leq n < 27, \\ \bar{F}(U_n^3(p_1, p_2, p_3)) = \bar{F}(U_n^3(p_1, p_2, 0)), & \text{for } n = 27, \\ \bar{F}(U_n^3(p_1, p_2, p_3)) < \bar{F}(U_n^3(p_1, p_2, 0)), & \text{for } n > 27. \end{cases} \quad (43)$$

Therefore, for $11 \leq n \leq 27$, $\bar{F}(U_n^3(p_1, p_2, p_3))$ has maximum F -coindex for the family of unicyclic graphs. $\square$

3. Conclusions

In this paper, we introduced an alternative form of F -coindex of graphs. We used this form to study different properties of unicyclic graphs. We also calculated maximum and minimum F -coindex for the family of unicyclic graphs.

This alternative form may be used to study F -coindex of some special and chemically interesting graphs. It may help in studying F -coindex of other classes of graphs like bicyclic and tricyclic classes. Furthermore, it would be an important direction if one can explore similar formula for other topological coindices.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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