South East Asian J. of Mathematics and Mathematical Sciences
Vol. 20, Proceedings (2022), pp. 215-226

ISSN (Online): 2582-0850

ISSN (Print): 0972-7752

ON THE KCD INDICES AND EXTREMAL GRAPHS

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(**Received:** *Apr. 08, 2022* **Accepted:** *Aug. 02, 2022* **Published:** *Aug. 30, 2022)*

Special Issue
Proceedings of National Conference on
"Emerging Trends in Discrete Mathematics, NCETDM - 2022"

Abstract: In this article, we present results on KCD indices related to extremal graphs of unicyclic graphs and characterize them in terms of diameter of graphs.

Keywords and Phrases: Extremal graphs, unicyclic graphs, KCD indices.

2020 Mathematics Subject Classification: 05C07, 05C12, 05C38.

1. Introduction

Graph theory, a very important part of chemical graph theory is used to model the properties of molecular structures. Cheminformatics, a merger of chemistry, mathematics and information science deals with the quantitative structure property relationships (QSPR) which has emerged as a tool in the medical and chemical field as it helps to predict the physico-chemical properties of compounds. In particular, this branch studies the physical and chemical properties of chemical compounds. These molecular structures are studied using a tool from graph theory. This affordable tool is the topological index. It is used to mathematically compute the value for a graph to characterize its topology. It forms a very important part of graph theory and is widely used in the fields of mathematical chemistry and chemical graph theory. Thus, topological indices of graph theory have gained wide acceptance as a tool to perform the analysis of molecular structures. A rich theory for topological indices is collected in [4, 5, 6, 8, 9]. They are classified as degree based and distance based topological indices. The first topological index evolved was Wiener index based on the distance concept and was defined by Wiener in 1947 to study the boiling points of alkanes. Later degree based topological indices were developed. The oldest degree based topological index was defined by Randić in 1975. Randić index $R(G)$ is [12]

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

Thereafter, another pair of degree based topological indices were defined by Gutman and named them as Zagreb indices came into existence [4, 5].
The first Zagreb index $M_1(G)$ i.e.,

$$M_1(G) = \sum_{uv \in E(G)} \left(d_G(u) + d_G(v)\right).$$

and second Zagreb index $M_2(G)$ i.e.,

$$M_2(G) = \sum_{uv \in E(G)} d_G(u)d_G(v).$$

These topological indices have attracted mathematicians for longer period as they have wide applications in the study of molecular structures. Many topological indices have been developed since then. For two graphs G and H, a graph G on n vertices having largest possible number of edges and not containing H as a subgraph is said to be an extremal graph [3]. The prime focus these days is to find the extremal results and extremal graphs for topological indices [1, 2, 13]. With this motivation we investigate some extremal results and extremal graphs for the recently defined KCD indices [10].

2. Preliminaries and Definitions

All the graphs considered in this paper are simple, connected and finite. For undefined terminologies we direct reader to [7].

Let G represent a graph with $|V(G)| = p$ and $|E(G)| = q$ as vertex and edge set respectively. $d_G(u)$ is the degree of a vertex u in G and $d_G(e) = d_G(u) + d_G(v) - 2$ is the edge degree. The distance of a vertex u to the farthest vertex in G is its diameter $D(G)$.

The KCD indices defined by Mirajkar et al. [10] are

$$KCD_1(G) = \sum_{e=uv \in E(G)} \left(\left(d_G(u) + d_G(v)\right) + d_G(e)\right) \tag{1}$$

$$KCD_2(G) = \sum_{e=uv \in E(G)} \Big(d_G(u) + d_G(v)\Big) d_G(e). \qquad (2)$$

Elaborated details for these concepts are available in [10, 11].

The graphs used for investigation are class of unicyclic graphs [1]. C_n is a cycle of order n, P_m is a path of size m and S_m is a star graph of size m.

For $n \geqslant 3, m \geqslant 3$ *and* $w \geqslant 1$, let $\bigcup = \{C_n, W(n,m,w), X(n,m,w), Y(n,m,w), Z(n,m,w)\}$ be the set of uncyclic graphs. The first member of the set $\bigcup$ is the cycle C_n. The next member is $W(n,m,w)$ representing a graph with a cycle C_n and w copies of P_m incident to a unique vertex of C_n. $X(n,m,w)$ is another member of $\bigcup$ consisting of w copies of P_m attached to each vertex of C_n. $Y(n,m,w)$ from $\bigcup$ denotes the graph with w copies of star graph S_m attached to only one vertex of C_n. The last member $Z(n,m,w)$ of $\bigcup$ is the graph with w copies of S_m incident to each vertex of C_n. The figure 1 depicts the members of $\bigcup$.

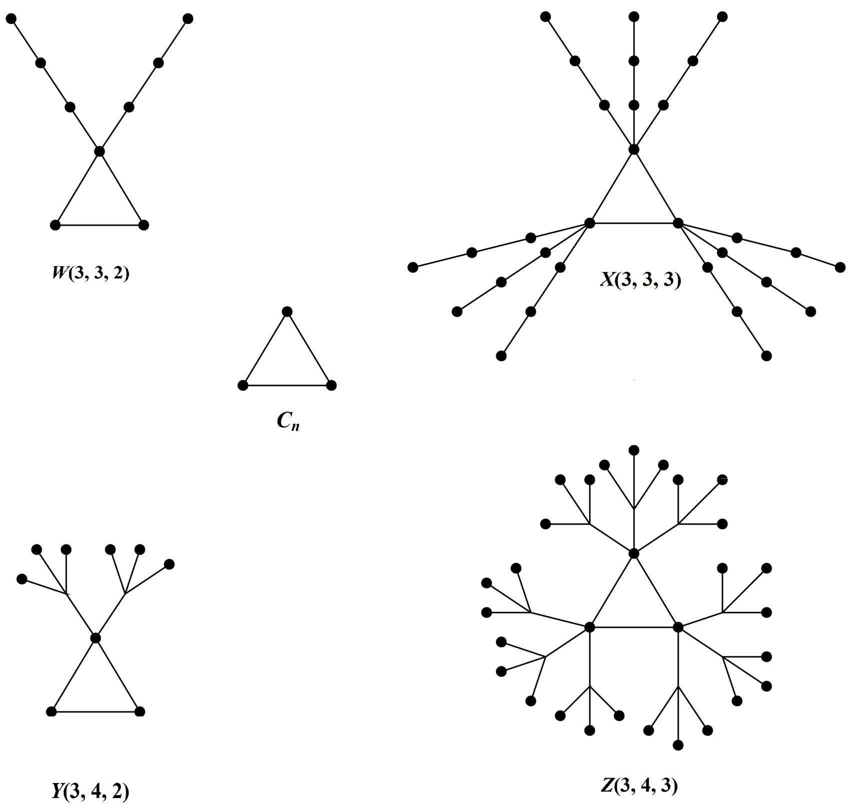

Figure 1: Unicyclic graphs of $\bigcup$.

3. Basic Results

Basic lemmas utilized in the proof of main results are proved in this section.

Lemma 3.1. *For integers $a \geqslant 3, b \geqslant 3$ and $c \geqslant 1$, the functions defined below*

1. $f_1(b,c) = -2c(c+3b+1)$
2. $g_1(b,c) = -2c(b^2+c+3)$
3. $h_1(a,b,c) = -2ac(3b+c+1)$
4. $l_1(a,b,c) = -2ac(b^2+c+3)$

are strictly decreasing.

Proof.

1. Due to the fact that,

$$\begin{aligned} \frac{\partial f_1}{\partial b} &= -6c < 0 \\ \textit{and } \frac{\partial f_1}{\partial c} &= -2(2c+3b+1) < 0 \end{aligned}$$

we conclude $f_1(b,c)$ as a strictly decreasing function (S. D. F.) for every $b \geqslant 3$ and $c \geqslant 1$.

2. Further,

$$\begin{aligned} \frac{\partial g_1}{\partial b} &= -4bc < 0 \\ \textit{and } \frac{\partial g_1}{\partial c} &= -2(2c+b^2+3) < 0 \end{aligned}$$

implying $g_1(b,c)$ is a S. D. F. for every $b \geqslant 3$ and $c \geqslant 1$.

3. Next,

$$\begin{aligned} \frac{\partial h_1}{\partial a} &= -2(c^2+3bc+c) < 0 \\ \frac{\partial h_1}{\partial b} &= -6ac < 0 \\ \textit{and } \frac{\partial h_1}{\partial c} &= -2(2ac+3ab+a) < 0 \end{aligned}$$

indicating $h_1(a,b,c)$ is a S. D. F. for every $a \geqslant 3, b \geqslant 3$ and $c \geqslant 1$.

4. Now,

$$\begin{aligned} \frac{\partial l_1}{\partial a} &= -2(cb^2+c^2+3c)<0 \\ \frac{\partial l_1}{\partial b} &= -4abc<0 \\ \textit{and}\ \ \frac{\partial l_1}{\partial c} &= -2(ab^2+2ac+3a)<0 \end{aligned}$$

this confirms $l_1(a,b,c)$ is a S. D. F. for every $a \geqslant 3, b \geqslant 3$ *and* $c \geqslant 1$.

Lemma 3.2. *For integers $a \geqslant 3, b \geqslant 3$ and $c \geqslant 1$, the functions defined below*

1. $f_2(b,c) = 2c(3b-b^2-2)$
2. $g_2(a,c) = (2c^2+6ac+2c)(1-a)$
3. $h_2(a,b,c) = 2c^2(1-a)+6c(b-a)+2c(1-ab^2)$

are strictly decreasing.

Proof.

1. Since,

$$\begin{aligned} \frac{\partial f_2}{\partial b} &= 6c-4cb<0 \\ \textit{and}\ \ \frac{\partial f_2}{\partial c} &= 6b-2b^2-4<0 \end{aligned}$$

this concludes that, $f_2(b,c)$ is a S. D. F. for every $b \geqslant 3$ *and* $c \geqslant 1$.

2. Also,

$$\begin{aligned} \frac{\partial g_2}{\partial a} &= 4c-2c^2-12ca<0 \\ \textit{and}\ \ \frac{\partial g_2}{\partial c} &= 4c+4a-4ac-6a^2+2<0 \end{aligned}$$

implying, $g_2(a,c)$ is a S. D. F. for every $a \geqslant 3$ *and* $c \geqslant 1$.

3. Next,

$$\begin{aligned} \frac{\partial h_2}{\partial a} &= -(2c^2+6c+2b^2c)<0 \\ \frac{\partial h_2}{\partial b} &= 6c-4abc<0 \\ \textit{and}\ \ \frac{\partial h_2}{\partial c} &= 4c-4ac+6b-6a+2-2ab^2<0 \end{aligned}$$

this implies, $h_2(a,b,c)$ is a S. D. F. for every $a \geqslant 3, b \geqslant 3$ *and* $c \geqslant 1$.

Lemma 3.3. *For integers $a \geqslant 3, b \geqslant 3$ and $c \geqslant 1$, the functions defined below*

$$\begin{array}{ll} 1. & f_3(a,b,c) = 2c^2(1-a) + 2cb(b-3a) + 2c(3-a) \\ 2. & g_3(a,b,c) = (2c^2 + 2cb^2 + 2c)(1-a) \end{array}$$

are strictly decreasing.

Proof.

1. Consider,

$$\begin{aligned} \frac{\partial f_3}{\partial a} &= -2(c^2 + 3bc + c) < 0 \\ \frac{\partial f_3}{\partial b} &= 4bc - 6ac < 0 \\ \text{and } \frac{\partial f_3}{\partial c} &= 4c - 4ac + 2b^2 - 6ab - 2a + 6 < 0 \end{aligned}$$

implying $f_3(a,b,c)$ is a S. D. F. for every $a \geqslant 3, b \geqslant 3$ *and* $c \geqslant 1$.

2. Since,

$$\begin{aligned} \frac{\partial g_3}{\partial a} &= -2(c^2 + b^2c + c) < 0 \\ \frac{\partial g_3}{\partial b} &= 4bc - 4abc < 0 \\ \text{and } \frac{\partial g_3}{\partial c} &= 4c + 2b^2 + 2 - 4ac - 4abc - 2a < 0 \end{aligned}$$

indicating $g_3(a,b,c)$ is a S. D. F. for every $a \geqslant 3, b \geqslant 3$ *and* $c \geqslant 1$.

Lemma 3.4. *For integers $a \geqslant 3, b \geqslant 3$ and $c \geqslant 1$, the function defined as*

$$f_4(a,b,c) = 2ac(3b - b^2 - 2)$$

is strictly decreasing.

Proof. Due to the fact that,

$$\begin{aligned} \frac{\partial f_4}{\partial a} &= 6bc - 2b^2c - 4c < 0 \\ \frac{\partial f_4}{\partial b} &= 6ac - 4abc < 0 \\ \text{and } \frac{\partial f_4}{\partial c} &= 6ab - 2ab^2 - 4a < 0 \end{aligned}$$

we conclude that, $f_4(a,b,c)$ is a S. D. F. for every $a \geqslant 3, b \geqslant 3$ *and* $c \geqslant 1$.

The KCD indices for the class of unicyclic graphs from $\bigcup$ are determined below.

Lemma 3.5. *For $n \geqslant 3, m \geqslant 3$ and $w \geqslant 1$, the first KCD index of unicyclic graphs are*

$$\begin{aligned} KCD_1(C_n) &= 6n && (3)\\ KCD_1(W(n,m,w)) &= 2\left(w^2+3wm+w+3n\right), m = D(P_m) && (4)\\ KCD_1(Y(n,m,w)) &= D(S_m)\left(w^2+wm^2+3w+3n\right) && (5)\\ KCD_1(X(n,m,w)) &= 2n\left(w^2+3wm+w+3\right), m = D(P_m) && (6)\\ \text{and } KCD_1(Z(n,m,w)) &= nD(S_m)\left(wm^2+w^2+3w+3\right). && (7)\end{aligned}$$

Proof. Proof follows from the definition of first KCD index given by Eq. 1.

Lemma 3.6. *For $n \geqslant 3, m \geqslant 3$ and $w \geqslant 1$, the second KCD index of unicyclic graphs are*

$$\begin{aligned} KCD_2(C_n) &= 8n && (8)\\ KCD_2(W(n,m,w)) &= w^3+8w^2+8wm+7w+8n, m = D(P_m) && (9)\\ KCD_2(Y(n,m,w)) &= wm^3+w^3+D(S_m)\left(w^2m+2w^2+4n\right)\\ &\quad +wm+13w. && (10)\end{aligned}$$

Proof. Proof follows from definition of second KCD index given by Eq. 2.

4. Main Results

In this section, we study the extremal unicyclic graphs from set $\bigcup$ and also obtain some extremal results in terms of diameter using KCD indices.

Theorem 4.1. *For $n \geqslant 3, m \geqslant 3$ and $w \geqslant 1$, the ordering of first KCD index among the members of $\bigcup$ is*

$$KCD_1(C_n) < KCD_1(W(n,m,w)) < KCD_1(Y(n,m,w)) < KCD_1(X(n,m,w)) < KCD_1(Z(n,m,w)).$$

Proof. The proof is developed in the form of Cases 1 to 4 using lemma 3.5 and the fact that $m = D(P_m)$ in Eqs. (4), (6) and $D(S_m) = 2$ for Eqs.(5), (7) as follows.

Case 1. Amongst the unicyclic graphs from the set $\bigcup$ the first minimum value for first KCD index is obtained for C_n.

Now,

$$KCD_1(C_n) - KCD_1(W(n,m,w)) = -2w(w+3m+1) \quad [\textit{using Eqs. (3) and (4)}]$$

By applying lemma 3.1 (1), we get

$$KCD_1(C_n) < KCD_1(W(n,m,w))$$

where $W(n,m,w)$ are the extremal unicyclic graphs for C_n.
Next,

$$KCD_1(C_n) - KCD_1(Y(n,m,w)) = -2w(w+m^2+3) \quad [\textit{using Eqs.}\ (3)\ \textit{and}\ (5)]$$

By applying lemma 3.1 (2), we get

$$KCD_1(C_n) < KCD_1(Y(n,m,w))$$

here Y(n,m,w) are the extremal unicyclic graphs for C_n.
Further,

$$KCD_1(C_n) - KCD_1(X(n,m,w)) = -2nw(w+3m+1) \quad [\textit{using Eqs.}\ (3)\ \textit{and}\ (6)]$$

By applying lemma 3.1 (3), we get

$$KCD_1(C_n) < KCD_1(X(n,m,w))$$

with X(n,m,w) being the extremal unicyclic graphs for C_n.
Lastly,

$$KCD_1(C_n) - KCD_1(Z(n,m,w)) = -2nw(m^2+w+3) \quad [\textit{using Eqs.}\ (3)\ \textit{and}\ (7)]$$

By applying lemma 3.1 (4), we get

$$KCD_1(C_n) < KCD_1(Z(n,m,w))$$

where $Z(n,m,w)$ are the extremal unicyclic graphs for C_n.

Thus , $KCD_1(C_n) < KCD_1(G)$ for every $G \in \bigcup - C_n$.

Case 2. The second minimum value for first KCD index amongst the members of $\bigcup$ is obtained by the comparision of $KCD_1(W(n,m,w))$ with first KCD index of remaining members of $\bigcup$ other than C_n.
Now,

$$KCD_1(W(n,m,w)) - KCD_1(Y(n,m,w)) = 6wm - 2wm^2 - 4w$$

$$[\text{using Eqs. (4) and (5)}]$$

By applying lemma 3.2 (1), we have

$$KCD_1(W(n,m,w)) < KCD_1(Y(n,m,w))$$

where Y(n,m,w) are the extremal unicyclic graphs for $W(n,m,w)$.
Next,

$$KCD_1(W(n,m,w)) - KCD_1(X(n,m,w)) \;=\; (2w^2+6wn+2w)(1-n)$$

[using Eqs. (4) and (6)]

By applying lemma 3.2 (2), we have

$$KCD_1(W(n,m,w)) < KCD_1(X(n,m,w))$$

with X(n,m,w) being the extremal unicyclic graphs for $W(n,m,w)$.
Finally,

$$KCD_1(W(n,m,w)) - KCD_1(Z(n,m,w)) = 2w^2(1-n) + 6w(m-n) + 2w(1-nm^2)$$

[using Eqs. (4) and (7)]

By applying lemma 3.2 (3), we have

$$KCD_1(W(n,m,w)) < KCD_1(Z(n,m,w))$$

here Z(n,m,w) are the extremal unicyclic graphs for $W(n,m,w)$.
Case 3. The third minimum value for first KCD index amongst the members of $\bigcup$ is acquired by comparing $KCD_1(Y(n,m,w))$ with first KCD index of $X(n,m,w)$ and $Z(n,m,w)$.
Now,

$$KCD_1(Y(n,m,w)) - KCD_1(X(n,m,w)) = 2w^2(1-n) + 2wm(m-3n) + 2w(3-n)$$

[using Eqs. (5) and (6)]

By using lemma 3.3 (1), gives

$$KCD_1(Y(n,m,w)) < KCD_1(X(n,m,w))$$

where X(n,m,w) are the extremal unicyclic graphs for $Y(n,m,w)$.
Also,

$$KCD_1(Y(n,m,w)) - KCD_1(Z(n,m,w)) \;=\; \left(2w^2+2wm^2+6w\right)(1-n)$$

[using Eqs. (5) and (7)]

By using lemma 3.3 (2), gives

$$KCD_1(Y(n,m,w)) < KCD_1(Z(n,m,w))$$

with Z(n,m,w) being the extremal unicyclic graphs for $Y(n,m,w)$.
Case 4. The fourth minimum value for first KCD index amongst the members of $\bigcup$ is acquired by comparing $KCD_1(X(n,m,w))$ with first KCD index of $Z(n,m,w)$.

Now,

$$KCD_1(X(n,m,w)) - KCD_1(Z(n,m,w)) = 2nw\left(3m - m^2 - 2\right)$$

[using Eqs. (6) and (7)]

By using lemma 3.4, we get

$$KCD_1(X(n,m,w)) < KCD_1(Z(n,m,w))$$

here Z(n,m,w) being the extremal unicyclic graphs for $X(n,m,w)$.
The discussions from Case 1 to Case 4 proves the theorem.

Theorem 4.2. *For $n \geqslant 3, m \geqslant 3$ and $w \geqslant 1$, the ordering of second KCD index among the members of $\bigcup$ is*

$$KCD_2(C_n) < KCD_2(W(n,m,w)) < KCD_2(Y(n,m,w)).$$

Proof. By considering similar arguments used to prove theorem 4.1 and using lemma 3.6 we obtain the required result.

Corollary 4.3. *For a graph G,*

$$KCD_1(G) - KCD_1(G-v) > 0 \text{ and } KCD_2(G) - KCD_2(G-v) > 0$$

Theorem 4.4. *For a tree T having order $n \geqslant 4$ and diameter $D(T)$*

$$KCD_1(T) \geqslant (5n-9) + D(T) \text{ and } KCD_1(T) \geqslant \left(\frac{2(3n-5)}{n-1}\right) D(T).$$

Proof. Let T be a tree.
For T to be a path, $KCD_1(T) = 6n - 10$ and $D(T) = n - 1$.
For T to be other than path, $D(T) \leqslant n - 2$ and T has minimum three vertices with degree 1. For longest path $P = v_0 v_1 ... v_D$ in T, it has at least one vertex u having degree 1 which is not present in P. Now, consider the deletion of the vertices having degree 1 not present in P from T, until T results into path P. We assume $u_1, u_2, ..., u_s$ to be the vertices in the Deleted order not present in P. By corollary 4.3 this results as

$$KCD_1(T) > KCD_1(T-u_1) > ... > KCD_1(T - \sum_{i=1}^{s} u_i) = KCD_1(P) = 6n - 10$$

$$D(T) = D(T - u_1) = ... = D(T - \sum_{i=1}^{s} u_i) = D(P).$$

Thus,

$$\begin{aligned} KCD_1(T) - D(T) &> KCD_1(P) - D(T) \\ &\geqslant (6n - 10) - (n - 1) \\ &\geqslant (5n - 9). \end{aligned} \tag{11}$$

and

$$\begin{aligned} \frac{KCD_1(T)}{D(T)} &> \frac{KCD_1(P)}{D(P)} \\ &\geqslant \frac{6n - 10}{n - 1} \\ &\geqslant \frac{2(3n - 5)}{n - 1}. \end{aligned} \tag{12}$$

simplification of inequalities (11) and (12) generates required results.

Theorem 4.5. *For a tree T having order $n \geqslant 4$ and diameter $D(T)$*

$$KCD_2(T) \geqslant (7n - 17) + D(T) \;\; \text{and} \;\; KCD_2(T) \geqslant \left(\frac{2(4n - 9)}{n - 1} \right) D(T).$$

Proof. By considering the definition of second KCD index defined in Eq. 2 and similar arguments used to prove theorem 4.4 we obtain the required results.

Remark 4.6. *Equality for theorems 4.4 and 4.5 is attained when T is a path. Further, path becomes extremal graph of star graph for these theorems.*

4. Conclusion

As the study of topological indices is mainly based on degree and distance concept of graphs, in this article we have examined some extremal results in terms of the diameter for class of extremal unicyclic graphs for KCD indices. However, class of bicyclic graphs, tricyclic graphs and others can be further studied as an open problem for these concepts.

5. Acknowledgement

Authors are thankful to Karnatak University, Dharwad, Karnataka, India for the support through University Research Studentship (URS), No.KU/Sch/URS/2020-21/1103 dated: 21/12/2020.

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