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Research Paper

On a Conjecture on Edge Mostar Index of Bicyclic Graphs

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Abstract

For an edge $e = uv$ of a graph G, $m_u(e|G)$ denotes the number of edges closer to the vertex u than to v (similarly $m_v(e|G)$). The edge Mostar index $Mo_e(G)$, of a graph G is defined as the sum of absolute differences between $m_u(e|G)$ and $m_v(e|G)$ over all edges $e = uv$ of G. H. Liu *et al.* proposed a conjecture on extremal bicyclic graphs with respect to the edge Mostar index [1]. Even though the conjecture was true in case of the lower bound and proved in [2], it was wrong for the upper bound. In this paper, we disprove the conjecture proposed by H. Liu *et al.* [1], propose its correct version and prove it. We also give an alternate proof for the lower bound of the edge Mostar index for bicyclic graphs with a given number of vertices.

1 Introduction

Topological indices are numerical quantities which are used to describe specific properties of graphs based on their structure. They are referred to as structural invariants, being structural parameters. The Wiener index [3], defined in 1947 by H. Wiener as a linear approximation of boiling points for paraffin molecules, is the first among these kinds of indices. A multitude of topological indices has been defined and extensively studied in chemical graph theory since its inception. In 2018, Tomislav Došlić *et al.* proposed Mostar index [4] as a measure to study the degree peripherality of edges and graphs [5]. Let $n_u(e|G)$ denote the number of vertices closer to u than to v (similarly for $n_v(e|G)$). Then, the Mostar index $Mo(G)$ of the graph $G = (V, E)$ is defined as

$$Mo(G) = \sum_{e=uv\in E} |n_u(e|G) - n_v(e|G)|.$$

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For a detailed literature on Mostar index, see [4–11]. Various modified versions of the Mostar index have been proposed and studied [5] during these years. One among them is the edge Mostar index. The edge Mostar index $Mo_e(G)$ [12] of the graph $G = (V, E)$ is defined as

$$Mo_e(G) = \sum_{e=uv \in E} |m_u(e|G) - m_v(e|G)|,$$

where $m_u(e|G)$ is the analogous edge version of $n_u(e|G)$. Since the outset of $Mo_e(G)$, few studies have been done on it. Arockiaraj *et al.* [12] determined the edge Mostar index for a family of coronoid and carbon nanocone structures. H. Liu *et al.* [1] determined the bounds of Mo_e for trees, unicyclic graphs, and cacti of a given order. In [13], M. Imran *et al.* determined the edge Mostar index of some chemical structures using graph operations. In [14], Nima Ghanbari *et al.* computed the edge Mostar index of some class of polymer graphs. Yasmeen *et al.* [15] computed the upper bound of the edge Mostar index for cacti with a fixed number of cycles. In [2], Ghalavand *et al.* determined the upper bound of the edge Mostar index for trees with a given diameter and the lower bound of the edge Mostar index for trees with some parameters.

Throughout this paper, we consider only simple, finite, undirected, connected graphs. A graph is bicyclic if it has exactly two induced cycles. A vertex v of a graph G is said to be a *pendant vertex* if its degree $d(v) = 1$ and the edge e incident on v is a *pendant edge*. In [1], H. Liu *et al.* proposed the following conjecture on the extremal bicyclic graphs with respect to the edge Mostar index.

Conjecture 1.1. *[1] If the size m of bicyclic graph is large enough, then $\Theta_{m-4,2,2}$ has the minimum edge Mostar index.*

Conjecture 1.2. *[1] If the size m of bicyclic graph is large enough, then the bicyclic graphs G_1 and G_2 (see Figure 1) have the maximum edge Mostar index.*

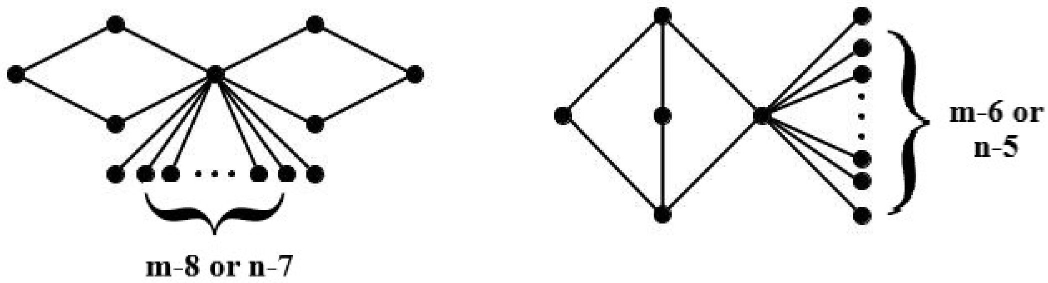

Figure 1: G_1 and G_2 of Conjecture 1.2.

Although Conjecture 1.1 was proved in [2], Conjecture 1.2 is not proved yet. Conjecture 1.2 proposed the existence of two graphs G_1 and G_2 attaining the upper bound of the edge Mostar index for bicyclic graphs, but we found that $Mo_e(G_1) - Mo_e(G_2) = 4 > 0$ for $n \geq 9$ (or size $m \geq 10$). In this paper, we propose and prove the correct version of the conjecture. We also give an alternate proof for Conjecture 1.1 in Section 4. For convenience, we state all the results in terms of the order of the graph.

2 Notations

For each edge $e = uv \in E$, let $\mu(e|G) = |m_u(e|G) - m_v(e|G)|$ denote the contribution by the edge e to the edge Mostar index.

Table 1: Notations and symbols.

$\mathcal{B}_n$	The collection of all bicyclic graphs of order n.
$\Theta_{a,b,c}$	The collection of all bicyclic graphs in which two vertices v_1 and v_2 are connected by three different paths of lengths a, b, c with $a \geq b \geq c$.
Θ_n	The collection of all bicyclic graphs in $\Theta_{a,b,c}$ with order n.
$\Phi_{a,b}$	The collection of all bicyclic graphs consisting of two cycles of lengths a and b without any common edges.
$\phi_{a,b,c}$	The bicyclic graph consisting of two cycles of lengths a and b together with c pendant edges attached at a common vertex u.
$\phi_{a,b}[T_1, T_2, \dots, T_m]$	The collection of all bicyclic graphs consisting of two distinct cycles C_a and C_b without any common edges along with tree T_i attached to some vertex u_i of C_a or C_b for $i = 1, 2, \dots, m$.
$\phi_{a,b}[S_1, S_2, \dots, S_r]$	The collection of all bicyclic graphs consisting of two distinct cycles C_a and C_b without any common edges in which the central vertex $v_i, (d(v_i) > 1)$ of the star graph S_i is identified with the vertex u_i of C_a or C_b for $i = 1, 2, \dots, r$.

3 Upper bound

In this section, we determine the upper bound of edge Mostar index of bicyclic graphs of order n.

Lemma 3.1. *[1] Let G be a graph with a cut edge $e = uv$ different from a pendant edge and G' is the graph obtained by contracting the edge e and adding a pendant edge $e' = wz$ at the contracting vertex w. Then*

$$Mo_e(G) < Mo_e(G').$$

Lemma 3.2. *Let $G \in \Phi_{a,b}$ be a bicyclic graph with n vertices, then $Mo_e(G) \leq Mo_e(\phi_{a,b,n+1-(a+b)})$.*

Proof. Let $G = \phi_{a,b}[T_1, T_2, \dots, T_r]$, using Lemma 3.1, we can say that

$$Mo_e(\phi_{a,b}[T_1, \dots, T_r]) \leq Mo_e(G'),$$

where $G' = \phi_{a,b}[S_1, S_2, \dots, S_r]$ with u be the vertex common to both C_a and C_b, $r = a + b - 1$. Now we will prove that $Mo_e(G') \leq Mo_e(G_1)$, where $G_1 = \phi_{a,b,n+1-(a+b)}$. For each edge e, let m_0^e denote the number of edges that are at an equal distance from the end vertices u and v other than the edge e and m_e denotes the diminishing factor in the contribution $\mu(e|G')$ without m_0^e.
Case I : a, b are even: For every edge $e \in C_a$, we have $\mu(e|G') = (n + 1 - m_e - m_0^e)$ where $m_e + m_0^e \geq a$, since every edge of C_a does not contribute to $\mu(e|G')$. For the corresponding edge in G_1, $\mu(e|G_1) = (n+1-a)$. Similarly for every edge $e \in C_b$, we have $\mu(e|G') = (n+1-m_e-m_0^e)$

where $m_e+m_0^e \geq b$ and $\mu(e|G_1) = (n+1-b)$. For every pendant edge e, $\mu(e|G') = n = \mu(e|G_1)$.

$$\begin{aligned}
Mo_e(G') - Mo_e(G_1) &= \sum_{e\in C_a} ((n+1-m_e-m_0^e) - (n+1-a)) \\
&+ \sum_{e\in C_b} ((n+1-m_e-m_0^e) - (n+1-b)) \\
&= \sum_{e\in C_a} (a-m_e-m_0^e) + \sum_{e\in C_b} (b-m_e-m_0^e) \leq 0.
\end{aligned}$$

Case II : a, b **are odd:** For every edge $e \in C_a$, we have $\mu(e|G') = (n+1-m_e-m_0^e)$ where $m_e \geq a$ and $m_0^e \geq 0$. For the corresponding edge in G_1, $\mu(e|G_1) = (n+1-a)$, except for one edge whose contribution $\mu(e|G_1) = 0$. Similarly, for every edge $f \in C_b$, $\mu(f|G') = (n+1-m_f-m_0^f)$ where $m_f \geq b$ and $\mu(f|G_1) = (n+1-b)$, except for one edge whose contribution $\mu(f|G_1) = 0$. For every pendant edge e, $\mu(e|G') = n = \mu(e|G_1)$.

$$\begin{aligned}
Mo_e(G') - Mo_e(G_1) &= \sum_{e\in C_a} (n+1-m_e-m_0^e) - \sum_{i=1}^{a-1}(n+1-a) \\
&+ \sum_{e\in C_b} (n+1-m_e-m_0^e) - \sum_{i=1}^{b-1}(n+1-b) \\
&= \sum_{i=1}^{a-1} (a-m_e) - \sum_{i=1}^{a} m_0^e + n+1-m_e \\
&+ \sum_{i=1}^{b-1} (b-m_e) - \sum_{i=1}^{b} m_0^e + n+1-m_e \\
&= \sum_{i=1}^{a} (a-m_e) + \sum_{i=1}^{b} (b-m_e) \leq 0.
\end{aligned}$$

Since $\sum_{i=1}^{a} m_0^e = n+1-a$ and $\sum_{i=1}^{b} m_0^f = n+1-b$.

Case III : a **odd and** b **even:** For every edge $e \in C_a$, we have $\mu(e|G') = (n+1-m_e-m_0^e)$, $m_e \geq a$. For the corresponding edge in G_1, $\mu(e|G_1) = (n+1-a)$ except for one edge whose contribution $\mu(e|G_1) = 0$. Similarly, for every edge $f \in C_b$ we have $\mu(f|G') = (n+1-m_f-m_0^f)$ where $m_f+m_0^f \geq b$. For the corresponding edge in G_1, $\mu(f|G_1) = (n+1-b)$. For every pendant edge e, $\mu(e|G') = n = \mu(e|G_1)$.

$$\begin{aligned}
Mo_e(G') - Mo_e(G_1) &= \sum_{e\in C_a} (n+1-m_e-m_0^e) - \sum_{i=1}^{a-1}(n+1-a) \\
&+ \sum_{e\in C_b} \Big((n+1-m_e-m_0^f) - (n+1-b)\Big) \\
&= \sum_{i=1}^{a-1} (a-m_e) - \sum_{i=1}^{a} m_0^e + n+1-m_e + \sum_{i=1}^{b} \Big(b-m_e-m_0^f\Big) \\
&= \sum_{i=1}^{a} (a-m_e) + \sum_{e\in C_b} \Big(b-m_e-m_0^f\Big) \leq 0.
\end{aligned}$$

Since $\sum_{i=1}^{a} m_0^e = n+1-a$. ■

Lemma 3.3. *Let $a, b \geq 4$ then,*

(a.) $Mo_e(\phi_{a,b,n+1-(a+b)}) \leq Mo_e(\phi_{a-2,b-2,n+5-(a+b)})$,

(b.) $Mo_e(\phi_{a,b,n+1-(a+b)}) \leq Mo_e(\phi_{a-2,b,n+3-(a+b)})$,

(c.) $Mo_e(\phi_{a,b,n+1-(a+b)}) \leq Mo_e(\phi_{a,b-2,n+3-(a+b)})$.

Proof. (a.) Let $G_1 = \phi_{a,b,n+1-(a+b)}$, $G_2 = \phi_{a-2,b-2,n+5-(a+b)}$ and u be the vertex common to both C_a and C_b. When a and b are even, for $a-2$ edges $e \in C_a$, we have $\mu(e|G_1) = n+1-a \leq \mu(e|G_2) = n+1-a+2$ and for the remaining two edges $e' \in C_a$, $\mu(e'|G_1) = n+1-a \leq \mu(e'|G_2) = n$. Similarly, for $b-2$ edges $e \in C_b$, $\mu(e|G_1) = n+1-b \leq \mu(e|G_2) = n+1-b+2$ and for the remaining two edges $e' \in C_b$, $\mu(e'|G_1) = n+1-b \leq \mu(e'|G_2) = n$. When a, b are odd, except for two edges, the contribution of edges is same as in the previous case. For two edges the contribution in both graphs is zero. When only a or b is odd, except for one edge whose contribution is zero, all the other edges have the same contribution as in the previous case. For each pendant edge, $\mu(e|G_1) = \mu(e|G_2)$. Thus for each edge e, $\mu(e|G_1) \leq \mu(e|G_2)$ hence $Mo_e(\phi_{a,b,n+1-(a+b)}) \leq Mo_e(\phi_{a-2,b-2,n+5-(a+b)})$.

(b.) Let $G_1 = \phi_{a,b,n+1-(a+b)}$ and $G_2 = \phi_{a-2,b,n+3-(a+b)}$. When a and b are even, for $a-2$ edges $e \in C_a$, we have $\mu(e|G_1) = n+1-a \leq \mu(e|G_2) = n+1-a+2$ and for the remaining two edges $e' \in C_a$, $\mu(e'|G_1) = n+1-a \leq \mu(e'|G_2) = n$. For every other edges, $\mu(e|G_1) = \mu(e|G_2)$. When a, b are odd, except for two edges, the contribution of edges is same as in the previous case. For two edges the contribution in both graphs is zero. When only a or b is odd, except for one edge whose contribution is zero all the other edges have the same contribution as in the previous case. For each pendant edge, $\mu(e|G_1) = \mu(e|G_2)$. Thus for each edge e, $\mu(e|G_1) \leq \mu(e|G_2)$ hence $Mo_e(\phi_{a,b,n+1-(a+b)}) \leq Mo_e(\phi_{a-2,b,n+3-(a+b)})$.

(c.) Proof is similar to Case (b).

■

Theorem 3.4. *Let $G \in \Phi_{a,b}$ be a bicyclic graph with order $n \geq 9$. Then $Mo_e(G) \leq n^2+n-24$ and the equality holds if and only if $G \cong \phi_{4,4,n-7}$.*

Proof. Let G be a bicyclic graph in $\Phi_{a,b}$ with maximum edge Mostar index. Then by Lemma 3.1, all the bridges of G are pendant edges and by Lemma 3.2, all the pendant edges of G should be at the common vertex. By Lemma 3.3, G can not have cycles of length more than 4. Thus G should be one among $\phi_{3,3,n-5}$, $\phi_{3,4,n-6}$ or $\phi_{4,4,n-7}$. In $\phi_{3,3,n-5}$, for $n-5$ pendant edges, $\mu(e|\phi_{3,3,n-5}) = n$, for two edges $\mu(e|\phi_{3,3,n-5}) = 0$ and for the rest of the four edges $\mu(e|\phi_{3,3,n-5}) = n-2$. Thus $Mo_e(\phi_{3,3,n-5}) = n^2-n-8$. Similarly, $Mo_e(\phi_{3,4,n-6}) = n^2-16$ and $Mo_e(\phi_{4,4,n-7}) = n^2+n-24$. Then clearly $Mo_e(\phi_{3,4,n-6}) > Mo_e(\phi_{3,3,n-5})$ and $Mo_e(\phi_{4,4,n-7}) > Mo_e(\phi_{3,4,n-6})$ for $n > 8$. ■

Let G be a graph with size m. Then for any edge $e = xy$ of G, $\mu(e|G) \leq m-1$ and the equality holds if and only if the edge is a pendant edge. For each edge $e \in G$, we define the *Deficiency* of the edge denoted by d_e as $d_e = m-1-\mu(e|G)$. *Deficiency* $D_e(G)$ of the graph G is the sum of the deficiencies over all of its edges and consequently $D_e(G) = \sum_{e \in G} d_e$. Clearly, $Mo_e(G) + D_e(G) = m(m-1)$. If $G \in \mathcal{B}_n$, then $Mo_e(G) + D_e(G) = n^2+n$. From the definition of *Deficiency* we have the following result.

Corollary 3.5. *Let G be any graph with a cycle C. Then for any edge $e \in C$, $d_e \geq 2$.*

Proof. For any edge $e = xy \in C$, there exist at least one edge in C closer to x than to y and at least one edge in C closer to y than to x. Thus $d_e \geq 2$. ■

By Theorem 3.4 we have the following result.

Corollary 3.6. *If G is a bicyclic graph on $n \geq 9$ vertices which attains the maximum edge Mostar index, then $D_e(G) \leq 24$.*

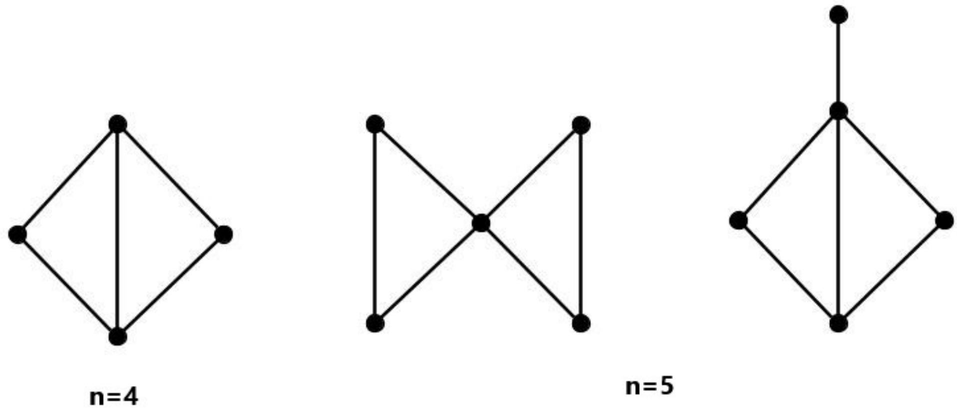

Figure 2: Bicyclic graphs with maximum Mo_e for orders 4,5.

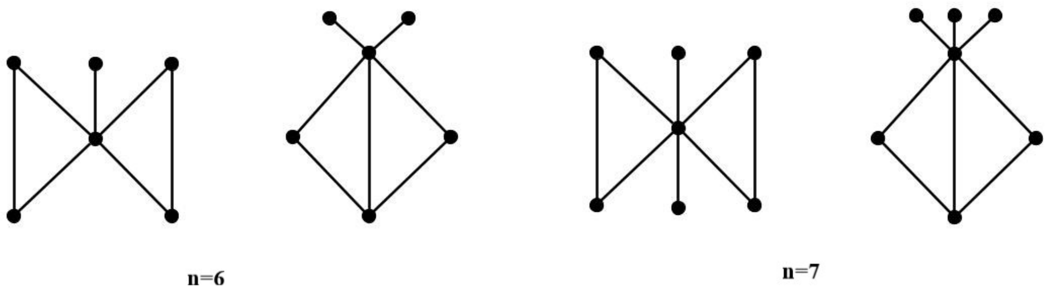

Figure 3: Bicyclic graphs with maximum Mo_e for orders 6,7.

Theorem 3.7. *Let $G \in \mathcal{B}_n$ be a bicyclic graph of order $n \geq 9$. Then $Mo_e(G) \leq n^2 + n - 24$ and the equality holds if and only if $G \cong \phi_{4,4,n-7}$.*

Proof. Let G be a bicyclic graph of order n. If $G \in \Phi_{a,b}$ then by Theorem 3.4 $Mo_e(G) \leq n^2 + n - 24$ and the maximum obtains if and only if $G \cong \phi_{4,4,n-7}$. Now, let $G \in \Theta_n$ be such that G attains maximum edge Mostar index, then by Corollary 3.6 $D_e(G) \leq 24$. Now, if $a+b+c \geq 13$ then by Corollary 3.5, $D_e(G) \geq 26$ which is not possible. Thus $a+b+c \leq 12$.

Now we consider the case when $a+b+c = 12$. In each of the subcases for possible values of a, b and c, there exist at least 7 edges such that $d_e \geq 6$. Thus $D_e(G) > 42$, impossible. When $a+b+c = 11$ or 10, in each of the cases, there exist at least 6 edges such that $d_e \geq 5$ and thus $D_e(G) > 30$. When $a+b+c = 9$, except for $a = 4, b = 4, c = 1$ in each of the other cases, there exist at least 6 edges such that $d_e \geq 5$ and thus $D_e(G) > 30$. Now for $a = 4, b = 4, c = 1$ there are 9 edges with $d_e \geq 4$ and thus $D_e(G) \geq 36$.

When $a+b+c = 8$, except for $a = 4, b = 3, c = 1$ and $a = 3, b = 3, c = 2$ in each of the other cases there are at least 6 edges such that $d_e \geq 5$ and hence $De(G) > 30$. For $a = 4, b = 3, c = 1$ there are 4 edges with $d_e \geq 4$ and 4 edges with $d_e \geq 3$ implying $D_e(G) \geq 28$. For $a = 3, b = 3, c = 2$ there are 8 edges with $d_e \geq 4$, thus $D_e(G) \geq 32$. When $a+b+c = 7$, except for $a = 3, b = 3, c = 1$ in each of the other cases there are at least 5 edges such that $d_e \geq 4$ and 2 edges with $d_e \geq 3$, thus $D_e(G) > 26$. For $a = 3, b = 3, c = 1$ there are at least 3 edges such that $d_e \geq 6$ and 4 edges with $d_e \geq 3$, thus $D_e(G) \geq 30$. When $a+b+c = 6$, for $a = 3, b = 2, c = 1$, $D_e(G) \geq n+17 \geq 26$, since $n \geq 9$. For $a = 2, b = 2, c = 2$, $D_e(G) \geq 28$. When $a+b+c = 5$, for $a = 2, b = 2, c = 1$, $D_e(G) = n+16 > 24$ since $n \geq 9$. Thus in each of these cases $Mo_e(G) \leq n^2+n-24$, hence the result. ■

As a consequence of the theorem, we have the following results.

Corollary 3.8. *Let $G \in \Theta_n$ be a bicyclic graph with order $n \geq 9$. Then $Mo_e(G) \leq n^2+n-28$ and equality holds if and only if $G \cong G'$ where G' is as in Figure 5.*

Thus, we have disproved the conjecture proposed by H. Liu. As per the conjecture, the graphs $\phi_{4,4,n-7}$ and G' attains the maximum edge Mostar index, but $Mo_e(\phi_{4,4,n-7}) = n^2+n-24$ and $Mo_e(G') = n^2+n-28$, clearly $Mo_e(\phi_{4,4,n-7}) > Mo_e(G')$. For graphs attaining maximum value of edge Mostar index among bicyclic graphs of order 4 to 8, see Figure 2, Figure 3, and Figure 4.

4 Lower bound

In this section, we give an alternate proof for the lower bound of the edge Mostar index of bicyclic graphs. For proving Theorem 4.3, we modify the methods described in [16].

Theorem 4.1. *For $n \geq 6$, $Mo_e(\Theta_{n-3,2,2}) = 2n-4$.*

Proof. When n is even, for $\frac{n-4}{2}$ edges of the path P_{n-2} closer to v_1 (as well as for v_2), $\mu(e|G) = 2$. For the $(\frac{n-4}{2}+1)-th$ edge of the path P_{n-2}, $\mu(e|G) = 0$ and for the rest of the edges $\mu(e|G) = 1$, thus $Mo_e(\Theta_{n-3,2,2}) = 2n-4$. When n is odd, for $\frac{n-5}{2}$ edges of the path P_{n-2} closer to v_1 (as well as for v_2), $\mu(e|G) = 2$ and for the rest of the edges $\mu(e|G) = 1$, thus $Mo_e(\Theta_{n-3,2,2}) = 2n-4$. ■

Corollary 4.2. *If G is a bicyclic graph with $n \geq 9$ vertices which attains the minimum value of edge Mostar index, then $Mo_e(G) \leq 2n-4$.*

Theorem 4.3. *Let $n \geq 9$, then $\Theta_{n-3,2,2}$ is the unique bicyclic graph with the minimum edge Mostar index.*

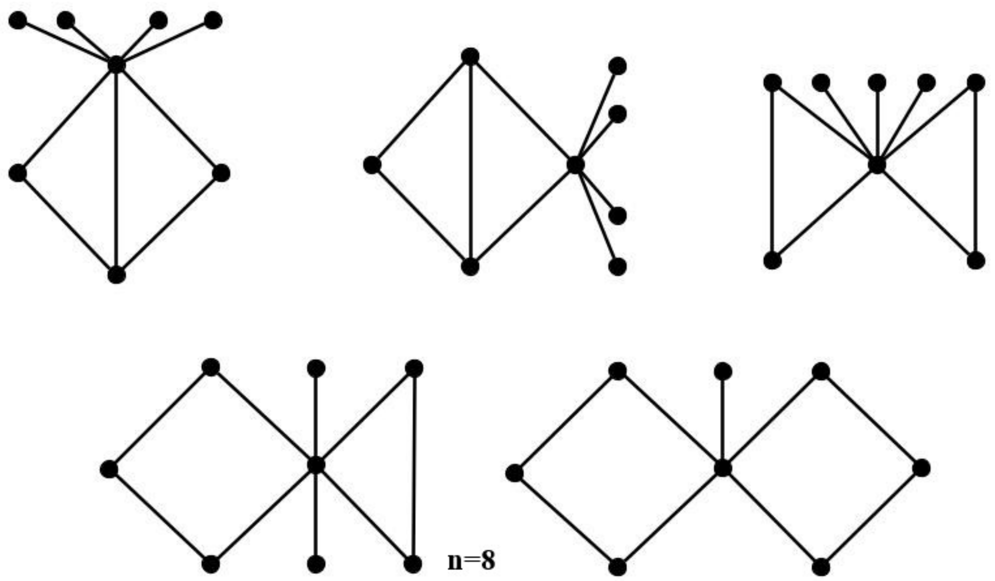

Figure 4: 8-vertex bicyclic graphs with the maximum edge Mostar index.

Proof. Let $G \in \mathcal{B}_n$ be the graph which attains minimum edge Mostar index. We prove the result using the following claims.

Claim I: G cannot have any pendant edges.

Consider the case that G has 2 or more pendant edges, then $\mu(e|G) = n$ for each one, thus $Mo_e(G) \geq 2n > 2n-4$ contradiction to Corollary 4.2. Thus G can not have more than one pendant edge, now consider the case that G has exactly one pendant edge e, then we have three different subcases:

Case IA: e is a pendant edge of a path of length 2 or more: If e is incident on a bridge e' which is not a part of the path connecting two cycles, then $\mu(e|G) + \mu(e'|G) \geq n + n - 2 = 2n - 2 > 2n - 4$, a contradiction. If e' is part of a path of length t connecting two cycles C_r, C_s, then there exist two edges each in C_r and C_s with $\mu(e|G) \geq n + 1 - r$ and $\mu(e|G) \geq n + 1 - s$ respectively, thus $Mo_e(G) \geq 4(n+1) - 2(r+s) + n \geq 3n + 4 > 2n - 4$, a contradiction.

Case IB: e is incident on a cycle where the two cycles have no common paths: Let G be the bicyclic graph having two different cycles C_r and C_s with $n = r + s + p, p \geq 0$, then there exist two edges each in C_r and C_s with $\mu(e|G) \geq s + p$ and $\mu(e|G) \geq r + p$ respectively. Thus $Mo_e(G) \geq 2(r + s + 2p) + n = 3n + 2p > 2n - 4$, a contradiction.

Case IC: e is incident on a cycle where the two cycles have common path: Let $G = \Theta_{a,b,c}$ with a pendant edge incident on some vertex of $\Theta_{a,b,c}$ where $n = a + b + c$. Then except for possibly three edges (one each in P_a, P_b, P_c,) for all the other edges e, $\mu(e|G) \geq 1$. Thus $Mo_e(G) \geq n + (a + b + c - 3) = 2n - 3 > 2n - 4$, a contradiction. Thus G cannot have any pendant edges.

Claim II: G cannot have any bridges.

Let e be a bridge of G, then e must be in the path of length t connecting two distinct cycles C_r and C_s(otherwise there must exist a pendant edge which is not possible), then $n = r + s + t - 1, t \geq 0$. As in Case IB, $Mo_e(G) \geq 2(r + s + 2t) = 2n + 2t - 2 > 2n - 4$, a contradiction. Thus G cannot have any bridges.

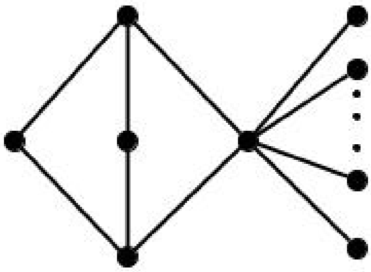

Figure 5: G' in Corollary 3.8.

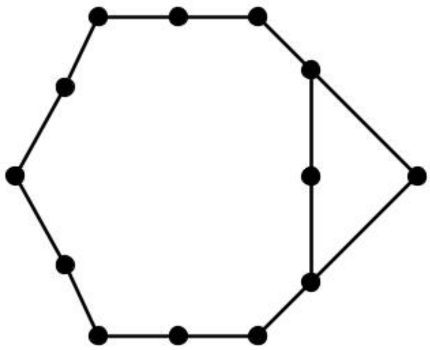

Figure 6: Bicyclic graph with smallest edge Mostar index of order 13.

Claim III: $G \in \Theta_{a,b,c}$.
Otherwise, suppose G contains two cycles which don't have a common path. By Claim II, G cannot have any bridges and hence in G the two cycles C_r and C_s must be identified at a single vertex u with $n = r + s - 1$. Also, there exist two edges e, e' of C_r incident with u and f, f' of C_s incident with u such that $\mu(e|G) \geq s$, $\mu(e'|G) \geq s$ and $\mu(f|G) \geq r$, $\mu(f'|G) \geq r$. Thus, $Mo_e(G) > 2(r + s) = 2n > 2n - 4$, a contradiction.
Thus G should be isomorphic to $\Theta_{a,b,c}$. Let w_1, w_2 be the vertices of degree 3 in G. According to the difference between a, b and c, we divide into nine possible cases.
Case III.1: $a = b = c$, here $n = 3a - 1$ the three edges incident at w_1 and w_2 each contribute at least $(a - 1)$ to Mo_e. Also, there is at least one other edge e such that $\mu(e|G) \geq 1$. Thus $Mo_e(G) \geq 6(a - 1) + 1 > 2n - 4$, a contradiction.
Case III.2: $a = b$ and $c = b - 1$. Two edges each incident at w_1 and w_2 contribute at least $(a-1)$ and one edge each incident at w_1 and w_2 contribute at least $(c-1)$. Also, there exist one more edge that contribute at least one. Thus $Mo_e(G) \geq (4a-4+2c-2)+1 = 2n-3 > 2n-4$ (since $n = 2a + c - 1$), a contradiction.
Case III.3: $a = b$ and $b > c + 1$. Two edges each incident at w_1 and w_2 contribute at least $(a-1)$ and one edge each incident at w_1 and w_2 contribute at least $(c-1)$. Also, there exist one more edge that contribute at least one. Thus $Mo_e(G) > (4a - 4 + c - 2) + 1 = 2n - 3 > 2n - 4$ (since $n = 2a + c - 1$), a contradiction.
Case III.4: $a = b + 1$ and $b = c$. Two edges each incident at w_1 and w_2 contribute at least

$(b-1)$ and one edge each incident at w_1 and w_2 contribute at least $(a-1)$. Also, there exist one more edge that contribute at least one. Thus $Mo_e(G) > (2a-2+4b-4)+1 = 2n-3 > 2n-4$ (since $n = a+2b-1$), a contradiction.

Case III.5: $a = b+1$ and $c = b-1$. Three edges each incident at w_1 and w_2 contribute at least $a-1$, b, $c-1$ respectively. Thus, $Mo_e(G) > (2a+2b+2c-4) = 2n-2 > 2n-4$ (since $n = a+b+c-1$), a contradiction.

Case III.6: $a = b+1$ and $b > c+1$. Three edges each incident at w_1 and w_2 contribute at least $a-1, b, c-1$ respectively. Also, there exist one more edge that contribute at least one. Thus $Mo_e(G) > 2a+2b+2c-3 = 2n-1 > 2n-4$ (since $n = a+b+c-1$), a contradiction.

Case III.7: $a > b+1$ and $c = b-1$. For each of the vertices w_1 and w_2, there are three edges incident at them which contribute at least $(b-1)$, $(c-1)$ and $\left(c + \left\lfloor \frac{a-b}{2} \right\rfloor\right)$ to $Mo_e(G)$ respectively. Also, there are $a-3$ edges that contribute at least one. Thus

$$Mo_e(G) \geq 2\left((b-1)+(c-1)+\left(c+\left\lfloor\frac{a-b}{2}\right\rfloor\right)\right)+a-3 > 2a+3b+2c-8 = 2n+b-6$$

and $2n+b-6 < 2n-4$ if $b \leq 2$. Now $b = 1$ is not possible. If $b = 2$, then $c = 1$ and $G = \Theta_{a,2,1}$. When $a \geq 4$ and $n = a+2$ is odd, then $Mo_e(G) = 3n-7$. $Mo_e(G) = 3n-7 < 2n-4$ whenever $n < 3$, a contradiction. When $a \geq 4$ and $n = a+2$ is even, $Mo_e(G) = 3n-8$, $Mo_e(G) = 3n-8 < 2n-4$ whenever $n < 4$, a contradiction.

Case III.8: $a > b+1$ and $b > c+1$. For each of the vertices w_1 and w_2 there are three edges each incident at them which contribute at least $a, b, c-1$ respectively. Thus $Mo_e(G) > 2a+2b+2c-2 = 2n > 2n-4$ (since $n = a+b+c-1$), a contradiction.

Case III.9: $a > b+1$ and $b = c$. $n = a+2b-1$, we divide it into four different cases. When a, b are even, i.e, n is odd. There are at least $a-4$ edges with $\mu(e|G) \geq 2$ and $2b-2$ edges with $\mu(e|G) \geq 1$. Also, there are two edges with $\mu(e|G) \geq b$ and four edges with $\mu(e|G) \geq b-1$, thus $Mo_e(G) \geq 2a+8b-14 = 2n+4b-12 > 2n-4$, when $b \geq 3$. When a is even and b is odd, i.e, n is odd. There are at least $a-3$ edges with $\mu(e|G) \geq 2$, $2b-5$ edges with $\mu(e|G) \geq 1$, two edges with $\mu(e|G) \geq b$, four edges with $\mu(e|G) \geq b-1$. Thus $Mo_e(G) \geq 2a+8b-15 = 2n+4b-13 > 2n-4$, when $b \geq 3$. When a is odd and b is even, i.e, n is even. There are at least $a-3$ edges with $\mu(e|G) \geq 2$, $2b-4$ edges with $\mu(e|G) \geq 1$, two edges with $\mu(e|G) \geq b$, four edges with $\mu(e|G) \geq b-1$. Thus $Mo_e(G) \geq 2a+8b-14 = 2n+4b-12 > 2n-4$, when $b \geq 3$. When a, b are odd, i.e, n is even. There are at least $a-3$ edges with $\mu(e|G) \geq 2$, $2b-6$ edges with $\mu(e|G) \geq 1$, two edges with $\mu(e|G) \geq b$, four edges with $\mu(e|G) \geq b-1$. Thus $Mo_e(G) \geq 2a+8b-16 = 2n+4b-14 > 2n-4$, when $b \geq 3$. Thus in all these cases $Mo_e(G) > 2n-4$ when $b \geq 3$, hence the only possibility is $b = 2$, i.e, $G = \Theta_{n-3,2,2}$. ■

Figure 6 is an example of a graph with smallest value of edge Mostar index among bicyclic graphs of order 13.

5 Concluding remarks

Edge Mostar index is a recently defined topological index as an extension of the Mostar index. In this paper, we have computed the extremum of the edge Mostar index for bicyclic graphs of a given order and characterized the graphs attaining the bounds and thus settled a Conjecture proposed in [1]. The computation of the edge Mostar index of various classes of molecular graphs is a problem that needs further research.

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