

## On Edge Mostar Index of Graphs

HECHAO LIU<sup>1,2</sup>, LING SONG<sup>1</sup>, QIQI XIAO<sup>1</sup> AND ZIKAI TANG<sup>1,\*</sup>

<sup>1</sup>School of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, P. R. China

<sup>2</sup>School of Mathematical Sciences, South China Normal University, Guangzhou, 510631, P. R. China

---

### ARTICLE INFO

---

#### Article History:

Received: 25 February 2020

Accepted: 20 April 2020

Published online: 30 July 2020

Academic Editor: Tomislav Došlić

---

#### Keywords:

Edge Mostar index

Tree

Unicyclic graph

Cacti

Extremal value

---



---

### ABSTRACT

---

The edge Mostar index  $Mo_e(G)$  of a connected graph  $G$  is defined as  $Mo_e(G) = \sum_{e=uv \in E(G)} |m_u(e|G) - m_v(e|G)|$ , where  $m_u(e|G)$  and  $m_v(e|G)$  are, respectively, the number of edges of  $G$  lying closer to vertex  $u$  than to vertex  $v$  and the number of edges of  $G$  lying closer to vertex  $v$  than to vertex  $u$ . In this paper, we determine the extremal values of edge Mostar index of some graphs. We characterize extremal trees, unicyclic graphs and determine the extremal graphs with maximum and second maximum edge Mostar index among cacti with size  $m$  and  $t$  cycles. At last, we give some open problems.

©2020 University of Kashan Press. All rights reserved

---

## 1. INTRODUCTION

In this paper, all graphs we consider are finite, undirected, and simple. Let  $G$  be a connected graph with vertex set  $V(G)$  and edge set  $E(G)$ . Let  $|G|$  and  $|E(G)|$  be the number of vertices and edges of  $G$ , respectively. For a vertex  $u \in V(G)$ , the degree of  $u$ , denoted by  $d_G(u)$  (or simply  $d(u)$ ), is the number of vertices which are adjacent to  $u$ . Call a vertex  $u$  a pendent vertex of  $G$ , if  $d(u) = 1$  and call an edge  $uv$  a pendent edge of  $G$ , if  $d(u) = 1$  or  $d(v) = 1$ .  $C_n$ ,  $S_n$  and  $P_n$  denote the cycle, star, and path with  $n$  vertices, respectively. For  $v \in V(G)$ , let  $G - v$  be a subgraph of  $G$  obtained by deleting vertex  $v$  and adjacent edges. For  $e \in E(G)$ , let  $G - e$  be a subgraph of  $G$  obtained by deleting edge  $e$ .

Among all the topological indices, the most well-known is the Wiener index [8], which is defined as the sum of distances over all unordered vertex pairs in  $G$ , namely

---

\*Corresponding Author (Email address: [zikaitang@163.com](mailto:zikaitang@163.com))

DOI: 10.22052/ijmc.2020.221320.1489

$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)$ . A long time known property of the Wiener index is the formula [8]

$$W(G) = \sum_{e=uv \in E(G)} n_u(e|G)n_v(e|G),$$

where  $n_u(e|G)$  and  $n_v(e|G)$  are, respectively, the number of vertices of  $G$  lying closer to vertex  $u$  than to vertex  $v$  and the number of vertices of  $G$  lying closer to vertex  $v$  than to vertex  $u$ . It is applicable for trees. Using the above formula, another topological index named the Szeged index [3], was introduced by Gutman, which is an extension of the Wiener index and defined by

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

Given an edge  $e = uv \in E(G)$ , the distance between the vertex  $x$  and the edge  $e$ , denoted by  $d(x, e)$ , is defined as  $d(x, e) = \min\{d(x, u), d(x, v)\}$ . Denote  $M_u(e|G) = \{e \in E(G) : d(u, e) < d(v, e)\}$  and  $M_v(e|G) = \{e \in E(G) : d(v, e) < d(u, e)\}$ . Let  $m_u(e|G) = |M_u(e|G)|$  and  $m_v(e|G) = |M_v(e|G)|$ . Then, the edge Szeged index [4] of  $G$  is defined as

$$Sz_e(G) = \sum_{e=uv \in E(G)} m_u(e|G)m_v(e|G).$$

Szeged index and edge Szeged index belongs to the class of bond-additive indices. Recently, another bond-additive topological index, named the Mostar index, has been introduced [2]. The Mostar index of a graph  $G$  is defined as

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

In [2], Došlić et al. proposed and investigated the Mostar index as a measure of peripherality in graphs. They determined its extremal values and characterized extremal trees and unicyclic graphs and gave a cut method for computing the Mostar index of benzenoid systems. In [6], Tepeh proved a conjecture of [2] on a characterization of bicyclic graphs with given number of vertices. One can refer [1,5,7] for more and some other details on the Mostar index.

The edge Mostar index [1] of a graph  $G$  is defined as

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

For the sake of simplicity, we consider the contribution  $\phi(e)$  of an edge  $e = uv$  defined as  $\phi(e) = |m_u(e|G) - m_v(e|G)|$ . The edge Mostar index is also one of the bond-additive indices. Edge Mostar index has also been introduced recently as a quantitative refinement of the distance nonbalancedness, and it can also measure peripherality of every edge and consider the contributions of all edges into a global measure of peripherality for a given chemical graph.

A connected graph is a cactus if any two cycles have at most one common vertex. A cycle in a cactus is called end-block if all but one vertex of the cycle have degree two. A bundle is a cactus that all cycles in the cactus have exactly one common vertex. Denoted by  $C(m, t)$  the class of all cactus with  $m$  edges in cycle and  $t$  cycles.

In this paper, we determine the extremal values of edge Mostar index of some graphs. We characterize extremal trees, unicyclic graphs and determine the extremal graphs with maximum and second maximum edge Mostar index among cacti with size  $m$  and  $t$  cycles. At last, we give some open problems.

## 2. PRELIMINARY RESULTS

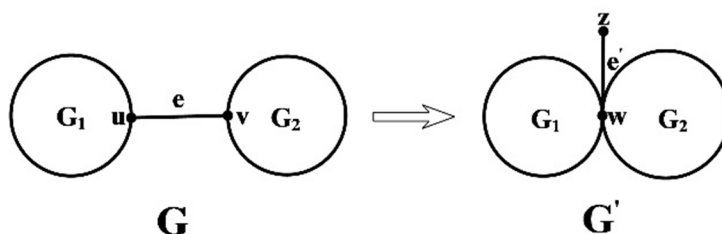
**Lemma 2.1.** *Let  $e = uv$  be a cut edge of connected graph  $G$ . Then*

$$\phi(e) = |m_u(e|G) - m_v(e|G)| \leq m - 1$$

*with equality if and only if  $e$  is a pendent edge.*

**Lemma 2.2.** (The edge-lifting transformation) *Let  $G$  be a graph with a cut, not pendent edge  $e = uv$ .  $G'$  is the graph obtained by contracting the edge  $e$  and adding a pendent edge  $e' = wz$  at the contracting vertex  $w$ , see Figure 1. Then  $Mo_e(G) < Mo_e(G')$ .*

**Proof.** From the definition of edge Mostar index, we know that  $\phi_G(e) \leq m - 3$  and  $\phi_{G'}(e) = m - 1$ . The contribution of other edges stays unchanged. Then  $Mo_e(G) - Mo_e(G') \leq -2 < 0$ . So,  $Mo_e(G) < Mo_e(G')$ . ■



**Figure 1.** The edge-lifting transformation.

## 3. THE EXTREMAL TREES AND UNICYCLIC GRAPHS

**Theorem 3.1.** *Let  $G$  be a tree with  $m$  ( $m \geq 4$ ) edges. Then*

$$Mo_e(P_{m+1}) < Mo_e(L_2) \leq Mo_e(G) \leq Mo_e(L_1) < Mo_e(S_{m+1}),$$

*for graphs  $L_1$  and  $L_2$  presented in Figure 2.*

**Proof.** Using the edge-lifting transformation of Lemma 2.2 repeatedly, we have that

$$Mo_e(G) \leq Mo_e(L_1) = m^2 - m - 2 < Mo_e(S_{m+1}) = m^2 - m.$$

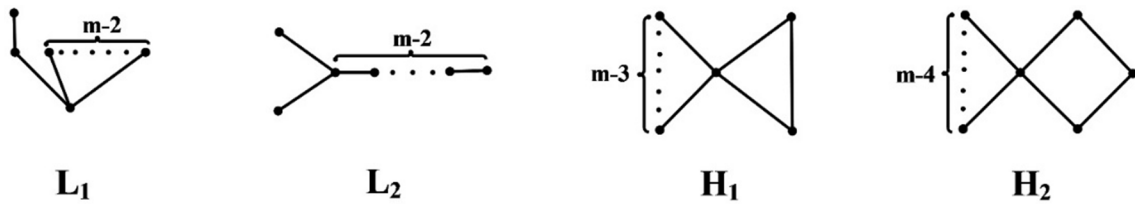
Suppose that  $G$  is a tree with  $m$  edges and  $G$  is not a path. Then, there exists a vertex  $z$  of degree at least three such that at least two components of  $G - z$  are paths. Denote the

two paths are  $P_s = u_1 u_2 \cdots u_s$  and  $P_t = v_1 v_2 \cdots v_t$  ( $1 \leq s \leq t$ ). Let  $G' = G - \{u_{s-1} u_s\} + \{v_t u_s\}$ . Then

$$\begin{aligned} Mo_e(G) - Mo_e(G') &= [(m-1) + (m-3) + \cdots + (m-2s+3) + (m-2s+1)] \\ &\quad + [(m-1) + (m-3) + \cdots + (m-2t+3) + (m-2t+1)] \\ &\quad - [(m-1) + (m-3) + \cdots + (m-2s+5) + (m-2s+3)] \\ &\quad - [(m-1) + (m-3) + \cdots + (m-2t+1) + (m-2t-1)] \\ &= 2(t-s) + 2 > 0. \end{aligned}$$

By computation, we have that  $Mo_e(P_{m+1}) = \frac{1}{2}m^2$  for  $m \equiv 0 \pmod{2}$ ;  $Mo_e(P_{m+1}) = \frac{1}{2}(m^2 - 1)$  for  $m \equiv 1 \pmod{2}$ . It means that  $Mo_e(P_{m+1}) = \lfloor \frac{1}{2}m^2 \rfloor$ .  $Mo_e(L_2) = \frac{1}{2}m^2 + 2$  for  $m \equiv 0 \pmod{2}$ ;  $Mo_e(L_2) = \frac{1}{2}(m^2 + 3)$  for  $m \equiv 1 \pmod{2}$ . It means that  $Mo_e(L_2) = \lfloor \frac{1}{2}m^2 \rfloor + 2$ . Such that  $Mo_e(G) \geq Mo_e(L_2) = \lfloor \frac{1}{2}m^2 \rfloor + 2 > Mo_e(P_{m+1}) = \lfloor \frac{1}{2}m^2 \rfloor$ .

The proof is completed. ■



**Figure 2.** The extremal trees and unicyclic graphs.

If  $G$  is a unicyclic graph, It is obvious that  $Mo_e(G) \geq Mo_e(C_m) = 0$ .

**Lemma 3.2.** *Let  $G$  be a unicyclic graphs with  $m$  edges, and the unique cycle  $C_g$ . Then*

$$Mo_e(G) \leq \begin{cases} (m-g)(m+g-1), & g \equiv 0 \pmod{2} \\ (m-g)(m+g+2), & g \equiv 1 \pmod{2} \end{cases},$$

with equality if and only if  $G$  is obtained from  $C_g$  by attaching  $m-g$  pendent edges at the same one vertex of  $C_g$ .

**Proof.** Suppose that  $G$  is a unicyclic graph with the unique cycle  $C_g = v_1 v_2 \cdots v_g v_1$ . Repeating the edge-lifting transformation of Lemma 2.2, the edge of  $E(G) \setminus E(C_g)$  are all pendent edge. Denote  $m_j$  ( $1 \leq j \leq g$ ) the number of pendent edges attached at  $v_j$ , then  $\sum_{j=1}^g m_j = m - g$ .

- i.  $g \equiv 0 \pmod{2}$ . For  $j \equiv 0 \pmod{g}$ ,  $\phi(v_j v_{j+1}) = \left| \sum_{k=1}^{\frac{g}{2}} m_{j+k} - \sum_{k=\frac{g}{2}+1}^g m_{j+k} \right| \leq \sum_{j=1}^g m_j = m - g$ . As the arbitrariness of  $j$ , the equality holds if and only if all

$m - g$  pendent edges attached at the same one vertex of  $C_g$ . Such  $\sum_{e \in E(G)} \phi(e) \leq (m - 1)(m - g) + (m - g)g = (m - g)(m + g - 1)$ , the equality holds if and only if all cut edges are pendent edges and all pendent edges attached at the same one vertex of  $C_g$ .

- ii.  $g \equiv 1 \pmod{2}$ . For  $j \equiv 1 \pmod{g}$ ,  $\phi(v_j v_{j+1}) = \left| \sum_{k=1}^{\frac{g-1}{2}} m_{j+k} - \sum_{k=\frac{g+3}{2}}^g m_{j+k} \right| \leq m - g - m_j$ . As the arbitrariness of  $j$ , the equality holds if and only if all  $m - g$  pendent edges attached at the same one vertex of  $C_g$ . Such  $\sum_{e \in E(G)} \phi(e) \leq (m - 1)(m - g) + (m - g)(g - 1) = (m - g)(m + g - 2)$ , the equality holds if and only if all cut edges are pendent edges and all pendent edges attached at the same one vertex of  $C_g$ .

The proof is completed. ■

**Theorem 3.3.** *Let  $G$  be a unicyclic graphs with  $m$  edges, then*

$$Mo_e(G) \leq \begin{cases} m^2 - 2m - 3, & 3 \leq m \leq 8 \\ 60, & m = 9 \\ m^2 - m - 12, & m \geq 10 \end{cases},$$

with equality if and only if  $G \cong H_1$  (see Figure 2) for  $3 \leq m \leq 8$ ;  $G \cong H_1$  or  $G \cong H_2$  for  $m = 9$ ;  $G \cong H_2$  (Figure 2) for  $m \geq 10$ .

**Proof.** By Lemma 3.2, if  $g \equiv 0 \pmod{2}$ , then  $Mo_e(G) \leq (m - g)(m + g - 1) \leq (m - 4)(m + 3) = m^2 - m - 12$ , with equality if and only if  $g = 4$  and all  $m - 4$  pendent edges attached at the same one vertex of  $C_4$ , i.e.  $G \cong H_2$ . If  $g \equiv 1 \pmod{2}$ , then  $Mo_e(G) \leq (m - g)(m + g - 2) \leq (m - 3)(m + 1) = m^2 - 2m - 3$ , with equality if and only if  $g = 3$  and all  $m - 3$  pendent edges attached at the same one vertex of  $C_3$ , i.e.  $G \cong H_1$ .

Comparing the edge Mostar index of  $H_1$  and  $H_2$ ,  $Mo_e(H_1) - Mo_e(H_2) = 9 - m$ . Such that, if  $3 \leq m \leq 8$ , then  $Mo_e(G) \leq m^2 - 2m - 3$  with equality if and only if  $G \cong H_1$ ; if  $m = 9$ , then  $Mo_e(G) \leq 60$  with equality if and only if  $G \cong H_1$  or  $G \cong H_2$ ; if  $m \geq 10$ , then  $Mo_e(G) \leq m^2 - m - 12$  with equality if and only if  $G \cong H_2$ .

The proof is completed. ■

#### 4. THE MAXIMUM VALUE OF EDGE MOSTAR INDEX AMONG CACTI

In the following, we give the sharp upper bounds of edge Mostar index among cacti.

**Lemma 4.1.** *Let  $G$  be a connected graph with a cycle  $C_g$  and  $G - E(C_g)$  has  $g$  connected components. Then*

$$\sum_{e=uv \in E(C_g)} \phi(e) \leq \begin{cases} g(m-g), & g \equiv 0 \pmod{2} \\ (g-1)(m-g), & g \equiv 1 \pmod{2} \end{cases},$$

with equality if and only if  $C_g$  is an end-block.

**Proof.** Let  $C_g = v_1 v_2 \cdots v_g v_1$ . Denoted by  $G_j$  the components of  $G - E(C_g)$  that contains  $v_j$  for  $1 \leq j \leq g$ . Let  $e_g = v_g v_1$  and  $e_{gj} = v_j v_{j+1}$  ( $1 \leq j \leq g-1$ ). Denote  $m_j = E(G_j)$ , then  $\sum_{j=1}^g m_j = m - g$ .

(i)  $g \equiv 0 \pmod{2}$ .

For  $e_g = v_g v_1 \in E(C_g)$ , we have that  $M_{v_1}(e) = E(G_1) \cup E(G_2) \cup \cdots \cup E(G_{\frac{g}{2}}) \cup \{e_1, e_2, \dots, e_{\frac{g}{2}-1}\}$  and  $M_{v_g}(e) = E(G_{\frac{g}{2}+1}) \cup E(G_{\frac{g}{2}+2}) \cup \cdots \cup E(G_g) \cup \{e_{\frac{g}{2}+1}, e_{\frac{g}{2}+2}, \dots, e_{g-1}\}$ .

If  $\sum_{j=1}^{\frac{g}{2}} m_j \geq \sum_{j=\frac{g}{2}+1}^g m_j$ , then

$$\phi(e) = \left| \sum_{j=1}^{\frac{g}{2}} m_j - \sum_{j=\frac{g}{2}+1}^g m_j \right| = \sum_{j=1}^{\frac{g}{2}} m_j - 2 \sum_{j=\frac{g}{2}+1}^g m_j \leq m - g,$$

equality holds if and only if  $m_j = 0$  for  $j = \frac{g}{2} + 1, \frac{g}{2} + 2, \dots, g$ . If  $\sum_{j=1}^{\frac{g}{2}} m_j \leq \sum_{j=\frac{g}{2}+1}^g m_j$ , then

$$\phi(e) = \left| \sum_{j=1}^{\frac{g}{2}} m_j - \sum_{j=\frac{g}{2}+1}^g m_j \right| = \sum_{j=1}^g m_j - 2 \sum_{j=1}^{\frac{g}{2}} m_j \leq m - g,$$

equality holds if and only if  $m_j = 0$  for  $j = 1, 2, \dots, \frac{g}{2}$ .

Similarly, we have that  $\phi(e_k) = |m_{v_k}(e_k) - m_{v_{k+1}}(e_k)| \leq m - g$  ( $1 \leq k \leq g-1$ ), equality holds if and only if  $m_j = 0$  for  $j = k - \frac{g}{2}, k - \frac{g}{2} + 1, \dots, k$  or  $m_j = 0$  for  $j = k + 1, k + 2, \dots, k + \frac{g}{2}$ , where  $j \equiv 0 \pmod{g}$ . Thus,  $\sum_{e=uv \in E(C_g)} \phi(e) \leq g(m-g)$ , with equality if and only if  $C_g$  is an end-block.

(ii)  $g \equiv 1 \pmod{2}$ .

For  $e_g = v_g v_1 \in E(C_g)$ , we have that  $M_{v_1}(e) = E(G_1) \cup E(G_2) \cup \cdots \cup E(G_{\frac{g-1}{2}}) \cup \{e_1, e_2, \dots, e_{\frac{g-1}{2}}\}$  and  $M_{v_g}(e) = E(G_{\frac{g+3}{2}}) \cup E(G_{\frac{g+5}{2}}) \cup \cdots \cup E(G_g) \cup \{e_{\frac{g+1}{2}}, e_{\frac{g+3}{2}}, \dots, e_{g-1}\}$ . If

$\sum_{j=1}^{\frac{g-1}{2}} m_j \geq \sum_{j=\frac{g+3}{2}}^g m_j$ , then

$$\phi(e) = \left| \sum_{j=1}^{\frac{g-1}{2}} m_j - \sum_{j=\frac{g+3}{2}}^g m_j \right| = \sum_{j=1}^g m_j - m_{\frac{g+1}{2}} - 2 \sum_{j=\frac{g+3}{2}}^g m_j \leq m - g - m_{\frac{g+1}{2}},$$

equality holds if and only if  $m_j = 0$  for  $j = \frac{g+3}{2}, \frac{g+5}{2}, \dots, g$ . If  $\sum_{j=1}^{\frac{g-1}{2}} m_j \leq \sum_{j=\frac{g+3}{2}}^g m_j$ , then

$$\phi(e) = \left| \sum_{j=1}^{\frac{g-1}{2}} m_j - \sum_{j=\frac{g+3}{2}}^g m_j \right| = \sum_{j=1}^g m_j - m_{\frac{g+1}{2}} - 2 \sum_{j=1}^{\frac{g-1}{2}} m_j \leq m - g - m_{\frac{g+1}{2}},$$

equality holds if and only if  $m_j = 0$  for  $j = 1, 2, \dots, \frac{g-1}{2}$ .

Similarly, we have that  $\phi(e_k) = |m_{v_k}(e_k) - m_{v_{k+1}}(e_k)| \leq m - g$  ( $1 \leq k \leq g - 1$ ), equality holds if and only if  $m_j = 0$  for  $j = k - \frac{g-3}{2}, k - \frac{g-5}{2}, \dots, k$  or  $m_j = 0$  for  $j = k + 1, k + 2, \dots, k + \frac{g-1}{2}$ , where  $j \equiv 0 \pmod{g}$ . Thus,

$$\sum_{e=uv \in E(C_g)} \phi(e) \leq \sum_{j=1}^g (m - g - m_j) \leq (g - 1)(m - g),$$

with equality if and only if  $C_g$  is an end-block.

So, the proof is completed.  $\blacksquare$

Denote  $G^m(g_1, g_2, \dots, g_t)$  a bundle of  $t$  cycles with lengths  $g_1, g_2, \dots, g_t$  and  $m - \sum_{j=1}^t g_j$  pendent edges attached to the unique common vertices of all cycles. Let  $\mathcal{G}_m$  be the set of  $G^m(g_1, g_2, \dots, g_t)$  with  $g_j = 3$  or  $g_j = 4$  for  $j = 1, 2, \dots, t$ .

**Lemma 4.2.** For any graph  $G \in \mathcal{C}(m, t)$ , suppose that  $C_1, C_2, \dots, C_t$  be the edge-disjoint cycles. Denote  $g_j = |C_j|$  for  $j = 1, 2, \dots, t$ , where  $g_j \equiv 1 \pmod{2}$  ( $j = 1, 2, \dots, r$ ) and  $g_j \equiv 0 \pmod{2}$  ( $j = r + 1, r + 2, \dots, t$ ). Then

$$Mo_e(G) \leq m^2 - m(r + 1) - \sum_{j=1}^r g_j (g_j - 2) - \sum_{j=r+1}^t g_j (g_j - 1),$$

with equality if and only if  $G \cong G^m(g_1, g_2, \dots, g_t)$ .

**Proof.** Denote  $E^*$  the set of all cut edge of  $G$ . Then  $E^* = E(G) \setminus \{\cup_{j=1}^t E(C_j)\}$  and  $|E^*| = m - \sum_{j=1}^t g_j$ . By Lemma 2.1, we have that  $\sum_{e \in E^*} \phi(e) \leq (m - 1)(m - \sum_{j=1}^t g_j)$ , with equality if and only if all cut edges are pendent edges.

By Lemma 4.1, we have that (1) If  $j = 1, 2, \dots, r$ , then  $\sum_{e \in E(C_j)} \phi(e) \leq (g_j - 1)(m - \sum_{j=1}^t g_j)$ , with equality if and only if  $C_j$  is an end-block. (2) If  $j = r + 1, r + 2, \dots, t$ , then  $\sum_{e \in E(C_j)} \phi(e) \leq g_j(m - \sum_{j=1}^t g_j)$ , with equality if and only if  $C_j$  is an end-block. With the definition of edge Mostar index, we have that

$$\begin{aligned} Mo_e(G) &\leq (m - 1)(m - \sum_{j=1}^t g_j) - \sum_{j=1}^r (g_j - 1)(m - g_j) - \sum_{j=r+1}^t g_j (m - g_j) \\ &= m(m - 1) - \sum_{j=1}^t g_j (m - 1) + \sum_{j=1}^r g_j (m - g_j) - \sum_{j=1}^r (m - g_j) \\ &= m(m - 1) - \sum_{j=1}^t g_j (g_j - 1) - \sum_{j=1}^r (m - g_j) \\ &= m^2 - m(r + 1) - \sum_{j=1}^r g_j (g_j - 2) - \sum_{j=r+1}^t g_j (g_j - 1), \end{aligned}$$

with equality if and only if all cut edges are pendent edges and all cycles are end-blocks, i.e.  $G \cong G^m(g_1, g_2, \dots, g_t)$ .

Hence, the proof is completed.  $\blacksquare$

**Theorem 4.3.** *Let  $G \in \mathcal{C}(m, t)$  be a connected graph. Then*

- (1) *If  $m \geq 10$  and  $m < 4t$ , then  $Mo_e(G) \leq 2m^2 - 8m + (24 - 4m)t$  with equality if and only if  $G \cong G^m(\underbrace{3, 3, \dots, 3}_{4t-m}, \underbrace{4, 4, \dots, 4}_{m-3t})$ .*
- (2) *If  $m \geq 10$  and  $m \geq 4t$ , then  $Mo_e(G) \leq m^2 - m - 12t$  with equality if and only if  $G \cong G^m(4, 4, \dots, 4)$ .*
- (3) *If  $m = 9$ , then  $Mo_e(G) = 72 - 12t$  with equality if and only if  $G \cong \mathcal{G}_9$ .*
- (4) *If  $m < 9$ , then  $Mo_e(G) \leq m^2 - m - (m + 3)t$  with equality if and only if  $G \cong G^m(3, 3, \dots, 3)$ .*

**Proof.** Suppose that  $C_1, C_2, \dots, C_t$  are  $t$  edge-disjoint cycles of  $G$  and  $g_j = |C_j|$  for  $j = 1, 2, \dots, t$ , where  $g_j \equiv 1 \pmod{2}$  ( $j = 1, 2, \dots, r$ ) and  $g_j \equiv 0 \pmod{2}$  ( $j = r + 1, r + 2, \dots, t$ ). By Lemma 4.2, we have that  $Mo_e(G) \leq Mo_e(G^m(g_1, g_2, \dots, g_t))$ . Let

$$\begin{aligned} f(g_1, g_2, \dots, g_t) &= Mo_e(G^m(g_1, g_2, \dots, g_t)) \\ &= m^2 - m(r + 1) - \sum_{j=1}^r g_j(g_j - 2) - \sum_{j=r+1}^t g_j(g_j - 1). \end{aligned}$$

Then  $\frac{\partial f(g_1, g_2, \dots, g_t)}{\partial g_j} = -4g_j - 1 < 0$ . So,  $f(g_1, g_2, \dots, g_t)$  is decreased for  $g_j$  ( $1 \leq j \leq t$ ).

Hence,  $f(g_1, g_2, \dots, g_t) \leq f(\underbrace{3, 3, \dots, 3}_r, \underbrace{4, 4, \dots, 4}_{t-r}) = m^2 - m - 12t - r(m - 9)$ .

Denote  $H(r) = m^2 - m - 12t - r(m - 9)$ ,  $H'(r) = 9 - m$ . Note that if  $m \geq 10$  and  $m - 4t < 0$ , then there are at least  $s$  triangles, where  $3s + 4(t - s) = m$ , i.e.,  $s = 4t - m > 0$ . So we have that

If  $m \geq 10$  and  $m < 4t$ , then  $H'(r) < 0$  and  $Mo_e(G) \leq H(4t - m) = 2m^2 - 8m + (24 - 4m)t$  with equality if and only if  $G \cong G^m(\underbrace{3, 3, \dots, 3}_{4t-m}, \underbrace{4, 4, \dots, 4}_{m-3t})$ .

If  $m \geq 10$  and  $m \geq 4t$ , then  $H'(r) < 0$  and  $Mo_e(G) \leq H(0) = m^2 - m - 12t$  with equality if and only if  $G \cong G^m(4, 4, \dots, 4)$ .

If  $m = 9$ , then  $H'(r) = 0$  and  $Mo_e(G) \leq f(g_1, g_2, \dots, g_t) \leq H(r) = 72 - 12t$  with equality if and only if  $G \cong \mathcal{G}_9$ .

If  $m < 9$ , then  $H'(r) > 0$  and  $Mo_e(G) \leq f(g_1, g_2, \dots, g_t) \leq H(r) \leq H(t) = m^2 - m - (m + 3)t$  with equality if and only if  $G \cong G^m(3, 3, \dots, 3)$ .

The proof is completed. ■

If  $t = 1$ ,  $\mathcal{C}(n, 1)$  is the set of unicyclic graphs. The maximum edge Mostar index among  $\mathcal{C}(n, 1)$  are determined, which is consistent with the result of the Theorem 3.3.



### 5. THE SECOND MAXIMUM VALUE OF EDGE MOSTAR INDEX AMONG CACTI

In the following, we will determine the unique graph in  $\mathcal{C}(m, t)$  with second maximum edge Mostar index. We assume that  $m \geq 10$  and  $m \geq 4t$ . Let

$$\mathcal{C}_0(m, t) \triangleq G^m(\underbrace{4, 4, \dots, 4}_t).$$

Denote  $\mathcal{C}_1(m, t)$  the graph that is obtained from  $\mathcal{C}_0(m - 1, t)$  by adding a pendent edge at a pendent vertex. If  $G \in \mathcal{C}(m, t) \setminus \{\mathcal{C}_0(m, t)\}$ , there are three possibilities:

- (1) There exists a cycle that is not  $C_4$ ;
- (2) There exists a cycle that is not an end-block;
- (3) There exists a cut edge that is not a pendent edge.

**Lemma 5.1.** *Let  $G \in \mathcal{C}(m, t) \setminus \{\mathcal{C}_0(m, t)\}$  with  $m \geq 10$ ,  $m \geq 4t$  and there exists a cycle that is not  $C_4$ . Then*

- (1) *If  $G$  has odd cycle, then  $Mo_e(G) \leq m^2 - 2m - 12t + 9$  with equality if and only if  $G \cong G^m(3, \underbrace{4, 4, \dots, 4}_{t-1})$ ;*
- (2) *If all cycle of  $G$  are even, then  $Mo_e(G) \leq m^2 - m - 12t - 18$  with equality if and only if  $G \cong G^m(6, \underbrace{4, 4, \dots, 4}_{t-1})$ .*

**Proof.** (1) If  $G$  has odd cycle, then  $r \geq 1$ . By Lemma 4.2 and Theorem 4.3, we have that

$$Mo_e(G) \leq f(g_1, g_2, \dots, g_t) \leq \underbrace{(3, 3, \dots, 3)}_r, \underbrace{4, 4, \dots, 4}_{t-r} \leq \underbrace{(3, 4, 4, \dots, 4)}_{t-1} = m^2 - 2m - 12t + 9,$$

with equality if and only if  $G \cong G^m(3, \underbrace{4, 4, \dots, 4}_{t-1})$ .

(2) If all cycle of  $G$  are even, then  $r = 0$ . By Lemma 4.2 and Theorem 4.3, we have that  $Mo_e(G) \leq f(g_1, g_2, \dots, g_t) \leq f(6, \underbrace{4, 4, \dots, 4}_{t-1}) = m^2 - m - 12t - 18$  with equality if and only if  $G \cong G^m(6, \underbrace{4, 4, \dots, 4}_{t-1})$ . The proof is completed. ■

**Lemma 5.2.** *Let  $G \in \mathcal{C}(m, t) \setminus \{\mathcal{C}_0(m, t)\}$  with  $m \geq 10$ ,  $m \geq 4t$  and there exists a cycle that is not an end-block. Then  $Mo_e(G) \leq m^2 - 2m - 12t + 9$  or  $Mo_e(G) \leq m^2 - m - 12t - 2$ .*

**Proof.** If there exists a cycle that is not  $C_4$ , then by Lemma 5.1, one knows that  $Mo_e(G) \leq m^2 - 2m - 12t + 9$  or  $Mo_e(G) \leq m^2 - m - 12t - 18$ . In the following, we assume that all cycles are  $C_4$  and  $C = v_1v_2v_3v_4v_1$  is not an end-block.

(1) If  $d(v_1) \geq 3$  and  $d(v_2) \geq 3$ , then

$$\sum_{e \in E(C)} \phi(e) \leq 2(m-4) + 2(m-6) = 4m - 20.$$

(2) If  $d(v_1) \geq 3$  and  $d(v_3) \geq 3$ , then  $\sum_{e \in E(C)} \phi(e) \leq 4(m-6) = 4m - 24 < 4m - 20$ .

Then

$$\begin{aligned} Mo_e(G) &\leq (m-1)(m-4t) + 4(m-4)(t-1) + 4m - 20 \\ &= m^2 - m - 12t - 4 \\ &< m^2 - m - 12t - 2. \end{aligned}$$

The proof is completed.  $\blacksquare$

**Lemma 5.3.** *Let  $G \in \mathcal{C}(m, t) \setminus \{\mathcal{C}_0(m, t)\}$  with  $m \geq 10$ ,  $m \geq 4t$  and there exists a cut edge that is not a pendent edge. Then  $Mo_e(G) \leq m^2 - m - 12t - 2$  with equality if and only if  $G \cong \mathcal{C}_1(m, t)$ .*

**Proof.** Suppose that  $e = uv$  is a cut edge that is not a pendent edge. Then  $1 \leq m_u(e), m_v(e) \leq m - 2$ , such  $\phi(e) \leq m - 3$  with equality if and only if one component of  $G - e$  contains a single edge. By Lemma 4.2 and Theorem 4.3, we have that

$$\begin{aligned} Mo_e(G) &\leq m - 3 + (m-1)(m - \sum_{j=1}^t g_j - 1) \\ &\quad + \sum_{j=1}^r (g_j - 1)(m - g_j) + \sum_{j=r+1}^t g_j (m - g_j) \\ &= f(g_1, g_2, \dots, g_t) - 2 \\ &\leq f(\underbrace{3, 3, \dots, 3}_r, \underbrace{4, 4, \dots, 4}_{t-r}) - 2 \\ &= m^2 - m - 12t - r(m-9) - 2 \\ &= H(r) - 2 \leq H(0) - 2 \\ &= m^2 - m - 12t - 2 \end{aligned}$$

with equality if and only if all cycles are  $C_4$  and end-block,  $e = uv$  is the only cut edge that is not a pendent edge, one component of  $G - e$  containing a single edge, i.e.  $G \cong \mathcal{C}_1(m, t)$ .

The proof is completed.  $\blacksquare$

By Lemma 5.1, 5.2, 5.3, we have the main result.

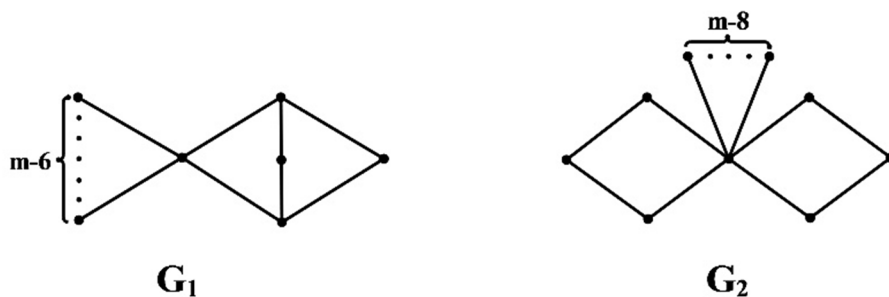
**Theorem 5.4.** *Let  $G \in \mathcal{C}(m, t) \setminus \{\mathcal{C}_0(m, t)\}$  with  $m \geq 10$ ,  $m \geq 4t > 0$ . Then*

(1)  $Mo_e(G) \leq 89 - 12t$  for  $m = 10$  with equality if and only if  $G \cong G(3, \underbrace{4, 4, \dots, 4}_{t-1})$ .

(2)  $Mo_e(G) \leq 108 - 12t$  for  $m = 11$  with equality if and only if  $G \cong G(3, \underbrace{4, 4, \dots, 4}_{t-1})$  or  $G \cong \mathcal{C}_1(m, t)$ .

(3)  $Mo_e(G) \leq m^2 - m - 12t - 2$  for  $m \geq 12$  with equality if and only if  $G \cong \mathcal{C}_1(m, t)$ .

Let  $\Theta_{a,b,c}$  be the Theta graph which is consisted by the three internally disjoint paths  $P_a, P_b, P_c$  of lengths  $a, b, c$ , respectively. If the bicyclic graphs are cacti, then through the results of Theorem 4.3 and 5.4, we can get the extremal graph. If there exists the Theta graph among bicyclic graphs, then we have the following conjectures.



**Figure 3.** The extremal bicyclic graphs  $G_1$  and  $G_2$ .

**Conjecture 5.5.** *If the size  $m$  of bicyclic graphs is large enough, then  $\Theta_{m-4,2,2}$  has the minimum edge Mostar index.*

**Conjecture 5.6.** *If the size  $m$  of bicyclic graphs is large enough, then the bicyclic graphs  $G_1$  and  $G_2$  (see Figure 3) have the maximum edge Mostar index.*

**ACKNOWLEDGEMENT.** Valuable comments and suggestions from the Editor and Reviewer are gratefully acknowledged. The research is supported by the Department of Education of Hunan Province(19A318), the National Natural Science Foundation of China (Grant No. 11971180), and the Guangdong Provincial Natural Science Foundation (Grant No. 2019A1515012052).

## REFERENCES

1. M. Arockiaraj, J. Clement and N. Tratnik, Mostar indices of carbon nanostructures and circumscribed donut benzenoid systems, *Int. J. Quantum Chem.* **119** (2019) e26043.
2. T. Došlić, I. Martinjak, R. Škrekovski, S. Tipurić Spužević and I. Zubac, Mostar index, *J. Math. Chem.* **56** (2018) 2995–3013.
3. I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y.* **27** (1994) 9–15.
4. I. Gutman and A. R. Ashrafi, The edge version of the Szeged index, *Croat. Chem. Acta* **81** (2008) 263–266.

5. F. Hayat and B. Zhou, On cacti with large Mostar index, *Filomat* **33** (2019) 4865–4873.
6. A. Tepeh, Extremal bicyclic graphs with respect to Mostar index, *Appl. Math. Comput.* **355** (2019) 319–324.
7. N. Tratnik, Computing the Mostar index in networks with applications to molecular graphs, *arXiv:1904.04131*.
8. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem.* **69** (1947) 17–20.