Research Article

Wiener Polarity Index of Cycle-Block Graphs

Zhen Jia, Fuyi Wei, and Yang Wu

Department of Mathematics, South China Agricultural University, Guangzhou 510642, China

Correspondence should be addressed to Fuyi Wei; weifuyi@scau.edu.cn

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The Wiener polarity index W_p of a graph G is the number of unordered pairs of vertices u, v of G such that the distance $d_G(u, v)$ between u and v is 3. Cycle-block graph is a connected graph in which every block is a cycle. In this paper, we determine the maximum and minimum Wiener polarity index of cycle-block graphs and describe their extremal graphs; the extremal graphs of 4-uniform cactus with respect to Wiener polarity index are also discussed.

1. Introduction

Let $G = (V, E)$ be a connected simple graph. The distance $d_G(u, v)$ between the vertices u and v of G is defined as the length of a shortest path connecting u and v . $N_G^i(u) = \{v \in V(G) \mid d_G(u, v) = i\}$ is called the i th neighbor set of u . $d(u) = |N_G^1(u)|$ is called the degree of u . If $d(u) = 1$, then u is called a pendant vertex of G . $C_l = u_1 u_2 \cdots u_l u_1$ denotes a cycle of order $l (\geq 3)$. The girth of G , denoted by g , is the length of the shortest cycle of G .

A block of the graph G is a maximal 2-connected subgraph of G . A cactus graph is a connected graph in which no edge lies in more than one cycle, such that each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles, the graph is defined as *cycle-block* graph. In this paper, suppose the cycle-block graph consist of n cycles, the length of the cycles may be different. If all blocks of a cactus G are cycles of the same length m , the cactus is *m-uniform*. A hexagonal cactus is a 6-uniform cactus that every block of the graph is a hexagon. A vertex shared by two or more hexagons is called a cut-vertex. If each hexagon of a hexagonal cactus G has at most two cut-vertices and each cut-vertex is shared by exactly two hexagons, we say that G is a chain hexagonal cactus (see Figure 1(a)). A star cactus is a cactus consisting of n cycles, spliced together in a single vertex u (see Figure 1(b)). A star hexagonal cactus is a star cactus in which every cycle is a hexagon.

The Wiener polarity index of G , denoted by $W_p(G)$, is the number of unordered vertex pairs of distance 3. It was first

used in a linear formula to calculate the boiling points t_B of paraffin [1]: of paraffin:

$$t_B = aW(G) + bW_p(G) + c, \quad (1)$$

where a, b, c are constants for a given isomeric group.

The Wiener polarity index became popular recently, and many mathematical properties and its chemical applications were discovered [2–6]. In this line, Du et al. [2] characterized the minimum and maximum Wiener polarity index among all trees of order n , and Deng [3] determined the largest Wiener polarity indices among all chemical trees of order n . M. H. Liu and B. L. Liu [4] determined the first two smallest Wiener polarity indices among all unicyclic graphs of order n . Hou et al. [5] determined the maximum Wiener polarity index of unicyclic graphs. Behmarama et al. [6] computed the Wiener polarity index of hexagonal cacti. To know more about cactus graph one can research [7, 8].

In this paper, we discuss the extremal graphs of Wiener polarity index of cycle-block graphs with $g \geq 5$ and 4-uniform cactus.

2. The Extremal Graphs of Wiener Polarity Index of Cycle-Block Graphs with $g \geq 5$

In this section, we characterize the maximum and minimum Wiener polarity index of the cycle-block graphs with $g \geq 5$.

Suppose that G_1 and G_2 are two connected graphs. The graph obtained by identifying a chosen vertex of G_1 and

FIGURE 1: A chain hexagonal cactus (a) and a star cactus graph (b).

another of G_2 is called the *coalescence* of G_1 and G_2 , denoted by $G_1 \circ G_2$. The vertex identifying G_1 and G_2 is called the *coalescence vertex*. The cycle-block graph which consist of n cycles $C_1, C_2, \dots, C_n$ can be seen as the coalescence of cycles by $n - 1$ times, $G \cong C_1 \circ C_2 \circ \dots \circ C_n$.

Lemma 1. Let G_1 and G_2 be two connected graphs; suppose that v_0 is the coalescence vertex of $G_1 \circ G_2$. Then $W_P(G_1 \circ G_2) = W_P(G_1) + W_P(G_2) + \sum_{k=1}^2 |N_{G_1}^k(v_0)| |N_{G_2}^{3-k}(v_0)|$.

Proof. Suppose that $u, v \in V(G_1 \circ G_2)$ and $d_{G_1 \circ G_2}(u, v) = 3$. Then,

$$\begin{aligned} & \left| \{(u, v) \mid d_{G_1 \circ G_2}(u, v) = 3, u, v \in V(G_i)\} \right| = W_P(G_i), \\ & \qquad \qquad \qquad i = 1, 2, \\ & \left| \{(u, v) \mid d_{G_1 \circ G_2}(u, v) = 3, u \in V(G_1), v \in V(G_2)\} \right| \\ & = \sum_{k=1}^2 |N_{G_1}^k(v_0)| |N_{G_2}^{3-k}(v_0)|. \end{aligned} \quad (2)$$

By the definition of Wiener polarity index, the result holds. $\square$

Theorem 2. Let G be a cycle-block graph with $g \geq 5$ and let G be consisting of n cycles $C_1, C_2, \dots, C_n$. Then

$$W_P(G) \leq \sum_{i=1}^n W_P(C_i) + 8 \binom{n}{2}; \quad (3)$$

the equality holds if and only if $G \cong G^*$, where G^* is a star cactus graph.

Proof. Let G be a cycle-block graph with $g \geq 5$. Here we apply induction to n .

When $k = 2$, the graph is determined uniquely. By Lemma 1 and elementary computation, we have $W_P(G) = \sum_{i=1}^2 W_P(C_i) + 8$.

When $k = 3$, there are three cycles C_1, C_2 , and C_3 . The graph G is obtained from $C_1 \circ C_2$ by attaching a new cycle C_3 to $C_1 \circ C_2$. There are three ways to attach the cycle C_3 . Here we suppose that v_0 is the coalescence vertex of $C_1 \circ C_2$ and v_1 is the new coalescence vertex of $C_1 \circ C_2 \circ C_3$.

By Lemma 1 and elementary computation, we have

$$W_P(G) = \begin{cases} \sum_{i=1}^3 W_P(C_i) + 8 \binom{3}{2}, & d(v_0, v_1) = 0, \\ \sum_{i=1}^3 W_P(C_i) + 20, & d(v_0, v_1) = 1, \\ \sum_{i=1}^3 W_P(C_i) + 16, & d(v_0, v_1) \geq 2, \end{cases} \quad (4)$$

where $d(v_0, v_1) = 0$ implies that G is the star cactus graph. From the result of the three cases, it holds for the result.

Now suppose that the assertion holds for $k = n - 1$. Next we prove that the result holds for $k = n$.

Suppose that v_0 is the coalescence vertex of $C_1 \circ C_2 \circ \dots \circ C_{n-1}$ and v_1 is the coalescence vertex of $C_1 \circ C_2 \circ \dots \circ C_n$. Three cases occur

$$W_P(G) = \begin{cases} \sum_{i=1}^n W_P(C_i) + 8 \binom{n}{2}, & d(v_0, v_1) = 0, \\ \sum_{i=1}^n W_P(C_i) + 8 \binom{n-1}{2} + 4n, & d(v_0, v_1) = 1, \\ \sum_{i=1}^n W_P(C_i) + 8 \binom{n-1}{2} + 8, & d(v_0, v_1) \geq 2, \end{cases} \quad (5)$$

where $d(v_0, v_1) = 0$; it implies that G is the star cactus graph. Obviously, the star cactus graph has the maximum Wiener polarity index of cycle-block graphs with $g \geq 5$. This completes the proof. $\square$

Let $\mathbb{G}$ be a graph set that consists of the cycle-block graphs of n cycles with $n-1$ cut-vertices and the distance between any cut-vertices being greater than 1. By a similar method with Theorem 2, we have Theorem 3; the proof is in the Appendix.

Theorem 3. Let G be a cycle-block graph with $g \geq 5$ and let G be consisting of n cycles $C_1, C_2, \dots, C_n$. Then

$$W_P(G) \geq \sum_{i=1}^n W_P(C_i) + 8(n-1); \quad (6)$$

the equality holds if and only if $G \in \mathbb{G}$.

Remark 4. By Theorems 2 and 3, we know that the cycle-block graph with maximum Wiener polarity index is determined

FIGURE 2: The graph of $Q_n(i, j, k, w)$.

uniquely while the cycle-block graph with minimum Wiener polarity index is not.

For some types of hexagonal cacti which represent common chemical structures, as an extension, we obtain the 6-uniform cactus with the maximum and minimum Wiener polarity index.

Corollary 5. Let G be 6-uniform cactus with n hexagons. Then $11n - 8 \leq W_P(G) \leq 4n^2 - n$; the first equality holds if and only if there are $n - 1$ different cut-vertices in G and distance between any two vertices is greater than 1; the second equality holds if and only if G is a star hexagonal cactus graph.

3. The Extremal Graphs of Wiener Polarity Index of 4-Uniform Cactus

The case of 4-uniform cactus' extremal graphs is different from the cycle-block graphs with $g \geq 5$ and more complex. Let $Q_n(i, j, t, w)$ be a graph obtained from a quadrilateral $C_4 = v_1 v_2 v_3 v_4 v_1$ by attaching i, j, t , and w quadrilaterals to vertices v_1, v_2, v_3 , and v_4 , respectively, where $i + j + t + w + 1 = n$ (see Figure 2).

Theorem 6. Suppose that G is 4-uniform with $n (\geq 2)$ quadrilaterals. Then

$$W_P(G) \leq 2n^2 - 2n; \quad (7)$$

the equality holds if and only if $G \cong Q_n(i, j, 0, 0)$, where $i \geq 0, j = n - 1 - i$.

Proof. We apply induction to n .

When $k = 2$, G is unique. By Lemma 1, we have $W_P(G) = 4$; the result follows.

When $k = 3$, we have

$$W_P(G) = \begin{cases} 12, & G \cong Q_3(2, 0, 0, 0), \\ 12, & G \cong Q_3(1, 1, 0, 0), \\ 8, & G \cong Q_3(1, 0, 1, 0); \end{cases} \quad (8)$$

the result holds.

Suppose that the result holds for $k = n - 1$. When $k = n$, there is a new quadrilateral to be attached to $Q_{n-1}(i, j, 0, 0)$,

where $j = n - 2 - i, i \geq 0$. Without loss of generality, suppose that $i > 0$; there are two cases to be discussed concerning of the variable parameters of j .

Case 1 ($j = 0$). It is a star quadrilateral cactus. Three new graphs $Q_n(n - 1, 0, 0, 0)$, $Q_n(n - 2, 1, 0, 0)$, and $Q_n(n - 2, 0, 1, 0)$ are obtained by three different ways to attach a quadrilateral to $Q_{n-1}(n - 2, 0, 0, 0)$.

By elementary computation and Lemma 1, we have

$$W_P(G) = \begin{cases} 2(n-1)^2 - 2(n-1) \\ \quad + 2 \times (n-1) + 1 \times 2(n-1), \\ 2(n-1)^2 - 2(n-1) \\ \quad + 2 \times (2(n-2) + 1) + 1 \times 2, \\ 2(n-1)^2 - 2(n-1) \\ \quad + 2 \times 1 + 1 \times 2, \end{cases} \quad (9)$$

$$= \begin{cases} 2n^2 - 2n, & G \cong Q_n(n-1, 0, 0, 0), \\ 2n^2 - 2n, & G \cong Q_n(n-2, 1, 0, 0), \\ 2n^2 - 6n + 8, & G \cong Q_n(n-2, 0, 1, 0). \end{cases}$$

For these three subcases, the result follows.

Case 2 ($j > 0$). There are also three subcases to attach a new quadrilateral to $Q_{n-1}(i, j, 0, 0)$.

Subcase 1. $G \cong Q_n(i + 1, j, 0, 0)$ or $G \cong Q_n(i, j + 1, 0, 0)$.

We only prove the case $G \cong Q_n(i + 1, j, 0, 0)$. $G \cong Q_n(i, j + 1, 0, 0)$ can be proved similarly. By elementary computation and Lemma 1, we have

$$\begin{aligned} W_P(Q_n(i + 1, j, 0, 0)) &= 2(n-1)^2 - 2(n-1) \\ &\quad + 2 \times (i + 1 + 2j) + 1 \times 2(i + 1) \\ &= 2n^2 - 2n. \end{aligned} \quad (10)$$

Subcase 2. $G \cong Q_n(i, j, 1, 0)$ or $G \cong Q_n(i, j, 0, 1)$.

When $G \cong Q_n(i, j, 1, 0)$, by elementary computation and Lemma 1, we have

$$\begin{aligned} W_P(Q_n(i, j, 1, 0)) &= 2(n-1)^2 - 2(n-1) + 2 \times (2j + 1) \\ &\quad + 1 \times 2 \\ &= 2n^2 - 6n + 4j + 8. \end{aligned} \quad (11)$$

Similarly, $W_P(Q_n(i, j, 0, 1)) = 2n^2 - 6n + 4i + 8$.

Subcase 3. The new quadrilateral attach to one of the i or j quadrilaterals and create a new cut-vertex different from v_1 and v_2 .

When a new quadrilateral is attached to one of the j quadrilaterals. The distance between the new cut-vertex and its nearest cut-vertex is 1. By elementary computation and Lemma 1, we have

$$\begin{aligned} W_P(G) &= 2(n-1)^2 - 2(n-1) + 2 \times (1 + 2j) + 1 \times 2 \\ &= 2n^2 - 6n + 4j + 8. \end{aligned} \quad (12)$$

FIGURE 3: The graph of G' .

Analogously, when the new quadrilateral is attached to one of the i quadrilaterals, we have $W_P(G) = 2n^2 - 6n + 4i + 8$.

When the distance between the new cut-vertex and its nearest cut-vertex is 2. By elementary computation and Lemma 1, we have

$$\begin{aligned} W_P(G) &= 2(n-1)^2 - 2(n-1) + 2 \times 1 + 1 \times 2 \\ &= 2n^2 - 6n + 8. \end{aligned} \quad (13)$$

By the discussion of Case 2 above, for $i > 0$, $j > 0$, it is easy to verify that $2n^2 - 2n > \max\{2n^2 - 6n + 4i + 12, 2n^2 - 6n + 4j + 12, 2n^2 - 6n + 8\}$. This completes the proof. $\square$

With the analogous method with Theorem 3, we can deduce the minimum Wiener polarity index of 4-uniform (see the proof of the Appendix).

Theorem 7. Let G be 4-uniform with n quadrilaterals. Then

$$W_P(G) \geq 4(n-1); \quad (14)$$

the equality holds if and only if $G \cong G'$, where G' is a chain quadrilateral cactus with the distance between the cut-vertices being at least 2 (see Figure 3).

Remark 8. From Theorems 6 and 7, we can conclude that the extremal 4-uniform with the maximum Wiener polarity index is not unique, but the minimum case is unique and different from the case of cycle-block graphs with $g \geq 5$. For the case of extremal cycle-block with $g \geq 3$ of Wiener polarity index is very complex, we do not discuss it here.

Appendix

The proof of Theorem 3.

Proof. We prove the result with the similar method of Theorem 2.

When $k = 2$, the graph is $C_1 \circ C_2$. By Lemma 1 and elementary computation, we have $W_P(G) = \sum_{i=1}^2 W_P(C_i) + 8$.

When $k = 3$, from the process of the proof of Theorem 2, Case 3 has the minimum Wiener polarity index. It holds for the result.

Suppose that $k = n - 1$ holds for the result; the smallest Wiener polarity index of cycle-block graphs is the cycle-block graph with $n - 2$ cut-vertex and any two cut-vertices' distance being greater than 1. Next we demonstrate that the result holds for $k = n$. There are four cases to be discussed. Suppose that $v_1, v_2, \dots, v_{n-2}$ are cut-vertices between

the cycles $C_1, C_2, \dots, C_{n-1}$. v_{n-1} is the cut-vertex of $C_1 \circ C_2 \circ \dots \circ C_n$. Consider the following:

$$W_P(G) = \begin{cases} \sum_{i=1}^{n-1} W_P(C_i) + 8(n-2) \\ \quad + W_P(C_n) + 2 \times 4 + 2 \times 4, \\ \sum_{i=1}^{n-1} W_P(C_i) + 8(n-2) \\ \quad + W_P(C_n) + 2 \times 6 + 2 \times 2, \\ \sum_{i=1}^{n-1} W_P(C_i) + 8(n-2) \\ \quad + W_P(C_n) + 2 \times 4 + 2 \times 2, \\ \sum_{i=1}^{n-1} W_P(C_i) + 8(n-2) \\ \quad + W_P(C_n) + 2 \times 2 + 2 \times 2, \end{cases}$$

$$= \begin{cases} \sum_{i=1}^n W_P(C_i) + 8n, & d(v_i, v_{n-1}) = 0, \\ & 1 \leq i \leq n-2, \\ \sum_{i=1}^n W_P(C_i) + 8n, & d(v_i, v_{n-1}) \\ & = d(v_j, v_{n-1}) = 1, \\ & 1 \leq i, j \leq n-2, i \neq j, \\ \sum_{i=1}^n W_P(C_i) + 8n-4, & d(v_j, v_{n-1}) = 1, \\ & d(v_i, v_{n-1}) > 1, \\ & 1 \leq i, j \leq n-2, i \neq j, \\ \sum_{i=1}^n W_P(C_i) + 8(n-1), & d(v_i, v_{n-1}) \geq 2, \\ & 1 \leq i \leq n-2. \end{cases} \quad (A.1)$$

From the discussion for $k = n$, we find that the result follows. By induction, it follows that the cycle-block graph $G \in \mathbb{G}$ has the minimum Wiener polarity index. $\square$

The proof of Theorem 7.

Proof. We prove the result with the same method of Theorem 3.

When $k = 2$ and $k = 3$, from the process of the proof of Theorem 6, it holds for the result.

Suppose that $k = n - 1$ holds for the result; next we prove the case of $k = n$ quadrilaterals. When $k = n$, it is the graph that by attaching a new quadrilateral to the chain quadrilateral cactus of $n - 1$ quadrilaterals which the distance between the cut-vertices is at least 2. There are four cases to be discussed. Suppose that $v_1, v_2, \dots, v_{n-2}$ are cut-vertices of the chain quadrilateral cactus with $n - 1$ quadrilaterals. v_{n-1} is the new coalescence vertex of $C_1 \circ C_2 \circ \dots \circ C_n$. Consider the following:

$$W_P(G) = \begin{cases} 4(n-2) + 2 \times 2 + 1 \times 4, \\ 4(n-2) + 2 \times 5 + 1 \times 2, \\ 4(n-2) + 2 \times 3 + 1 \times 2, \\ 4(n-2) + 2 \times 1 + 1 \times 2, \end{cases}$$

$$= \begin{cases} 4n, & d(v_i, v_{n-1}) = 0, \\ & 1 \leq i \leq n-2, \\ 4n+4, & d(v_i, v_{n-1}) = d(v_j, v_{n-1}) = 1, \\ & 1 \leq i, j \leq n-2, i \neq j, \\ 4n, & d(v_j, v_{n-1}) = 1, d(v_i, v_{n-1}) > 1, \\ & 1 \leq i, j \leq n-2, i \neq j, \\ 4(n-1), & d(v_i, v_{n-1}) \geq 2, \\ & 1 \leq i \leq n-2. \end{cases} \quad (\text{A.2})$$

When $d(v_i, v_{n-1}) \geq 2, 1 \leq i \leq n-2$, graph G is the chain quadrilateral cactus of $n-1$ quadrilaterals with the distance between the cut-vertices being at least 2; the result follows. By induction, it follows that the chain quadrilateral cactus with the distance between the cut-vertices being at least 2 has the minimum Wiener polarity index. This completes the proof. $\square$

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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