Research Article

Some new results on the reciprocal complementary Wiener number of graphs

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Abstract

The reciprocal complementary Wiener number of a graph is one of the applied distance-based topological indices. For a connected graph G, this topological index is defined as the sum of the weights $(D + 1 - d_G(x, y))^{-1}$ over all unordered pairs of vertices x and y of G, where D is the diameter of G and $d_G(x, y)$ denotes the distance (that is equal to the length of a shortest path) between x and y. In this paper, the reciprocal complementary Wiener number of some cactus graphs is studied.

Keywords: reciprocal complementary Wiener number; distance in graphs; cactus chains.

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1. Introduction and preliminaries

In the mathematical chemistry literature, a molecular descriptor that is calculated from the molecular graph of a chemical compound is known as a topological index. Most of the well-studied topological indices are based on the distances between vertices or/and the degrees of vertices of the molecular graph. The Wiener index is the oldest distance-based topological index and is one of the most-studied topological indices, both from the theoretical point of view as well as from the applications point of view [11]. The first and second Zagreb indices are among the oldest degree-based topological indices [2, 3].

Let G be a graph with the vertex set $V(G) = \{x_1, x_2, \ldots, x_n\}$ and diameter D. The *reciprocal complementary distance matrix* $RCD = [rc_{ij}]$ of G is an $n \times n$ matrix such that

$$rc_{ij} = \frac{1}{D + 1 - d_G(x_i, x_j)} \quad \text{if} \quad i \neq j,$$

and 0 otherwise (see [6]). Ivanciuc et al. [4, 5] defined the *reciprocal complementary Wiener number* of the gragh G as:

$$RCW(G) = \sum_{1 \leq i < j \leq n} rc_{ij} = \sum_{\{x_i, x_j\} \subseteq V(G)} \frac{1}{D + 1 - d_G(x_i, x_j)}. \tag{1}$$

If $d(G, k)$ is the number of vertex pairs at distance k in the graph G, then we have

$$RCW(G) = \sum_{k=1}^{D} \frac{d(G, k)}{D + 1 - k}. \tag{2}$$

This concept has been successfully applied in the structure-property modeling of the molar heat capacity, standard Gibbs energy of formation and vaporization enthalpy of 134 alkanes C_6-C_{10} (see [4]). Recently, we studied the reciprocal complementary Wiener number of various graph operations like join, Cartesian product, composition, strong product, disjunction, symmetric difference, corona product, splice and link of graphs [8]. In [7], we established some new bounds for the reciprocal complementary Wiener number of graphs in terms of the diameter, first and second Zagreb indices, Wiener number, number of vertices, edges and hexagons of graphs. The trees with the smallest, second smallest and third smallest RCW, and the unicyclic and bicyclic graphs with the smallest and second smallest RCW were determined in [1]. Zhou et al. [12] gave some properties for the reciprocal complementary Wiener number, especially various upper and lower bounds and a Nordhaus-Gaddum-type result for this invariant. For $4 \leq D \leq n - 3$, the unique tree with the minimum reciprocal complementary Wiener number, and the non-caterpillars with the first three smallest values of the reciprocal complementary Wiener number were characterized in [13]. Moreover, Ramane et al. [9] presented some bounds on RCW for line graphs.

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A *cactus graph* is a connected graph in which any two of its cycles have at most one common vertex. Consequently, each block of this graph is either an edge or a cycle. If all the blocks of a cactus G are cycles of the same size l, the cactus is l-uniform. A *triangular cactus* is a 3-uniform cactus, i.e., a cactus in which every block is a triangle. If no triangle of a triangular cactus G has more than two cut vertices, and each cut vertex is shared by exactly two triangle, we say that G is a *chain triangular cactus*. We denote by $\mathcal{T}_n$ the chain triangular cactus graph with n triangles (see Figure 1). By replacing the cycles C_3 in the chain triangular cactus $\mathcal{T}_n$ with the cycles C_4 we obtain cactus graph known as the *square cactus chain*. The *Para-chain square cactus graph*, denoted by $\mathcal{Q}_n$, is a square cactus chain in which the cut vertices of each of its internal squares are not adjacent (see Figure 2). Also, if the cut vertices of each internal squares of a square cactus chain are adjacent then we call it as the *Ortho-chain square cactus graph* and denote it by $\mathcal{O}_n$ (see Figure 3). Similarly, the *chain hexagonal cactus* are obtained by replacing the cycles C_3 with the cycles C_6 in the chain triangular cactus $\mathcal{T}_n$. The *Para-chain hexagonal cactus graph*, denoted by $\mathcal{L}_n$, is a chain hexagonal cactus in which the cut vertices of each of its internal hexagons are at distance three (see Figure 4). Also, if the cut vertices of each of the internal hexagons of a chain hexagonal cactus are at distance two then we call it as the *Meta-chain hexagonal cactus graph* and denote it by $\mathcal{M}_n$ (see Figure 5).

In this paper, we continue our research on the reciprocal complementary Wiener number by determining its values for the above-mentioned cactus chain graphs.
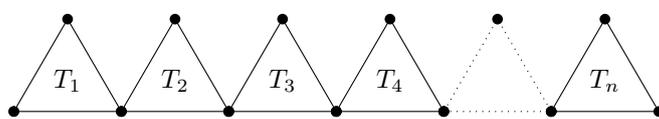

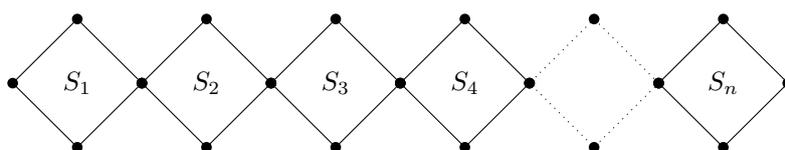
Figure 1: The chain triangular cactus graph $\mathcal{T}_n$.

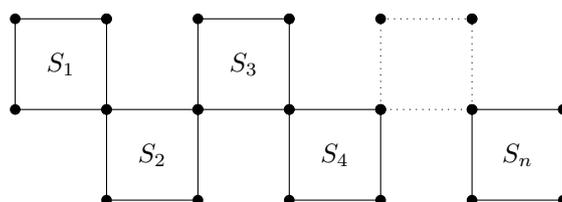Figure 2: The Para-chain square cactus graph $\mathcal{Q}_n$.

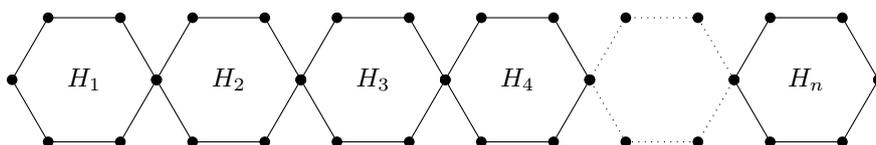Figure 3: The Ortho-chain square cactus graph $\mathcal{O}_n$.

Figure 4: The Para-chain hexagonal cactus graph $\mathcal{L}_n$.
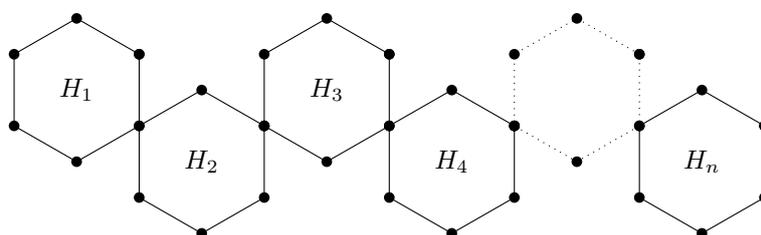

Figure 5: The Meta-chain hexagonal cactus graph $\mathcal{M}_n$.

2. Main results

In this section, we study the reciprocal complementary Wiener number of the chain triangular cactus graph, two types of the square cactus chains and two kind of the hexagonal cactus chains.

Theorem 2.1. *If $\mathcal{T}_n$ $(n \geq 2)$ is the chain triangular cactus graph, then*

$$RCW(\mathcal{T}_n) = 4n - 1.$$

Proof. By [10], we have

$$
d(\mathcal{T}_n, k) = \begin{cases} 3n & k = 1, \\ 4 & k = n, \\ 4n - 4k + 4 & 2 \leq k \leq n - 1. \end{cases}
$$

Therefore,

$$RCW(\mathcal{T}_n) = \sum_{k=1}^{D=n} \frac{d(\mathcal{T}_n, k)}{n + 1 - k} = 7 + \sum_{k=2}^{n-1} \frac{4n - 4k + 4}{n + 1 - k} = 4n - 1.$$

$\square$

Theorem 2.2. *Let $\mathcal{Q}_n$ $(n \geq 2)$ and $\mathcal{O}_n$ $(n \geq 5)$ be the Para-chain and Ortho-chain square cactus graphs, respectively.*

(i). *For $\mathcal{Q}_n$, it holds that*

$$RCW(\mathcal{Q}_n) = \frac{18n^2 - 13n}{4n - 2} - \frac{3}{2} \sum_{k=1}^{n-2} \frac{1}{2k + 1}.$$

(ii). *For $\mathcal{O}_n$, it holds that*

$$RCW(\mathcal{O}_n) = 9n - 9 - \frac{30n^2 + 64n + 24}{n^3 + 3n^2 + 2n} - 12 \sum_{k=4}^{n-1} \frac{1}{k}.$$

Proof. By [10], we have

$$
d(\mathcal{Q}_n, k) = \begin{cases} 6n - 4 & k = 2, \\ 4 & k = 2n - 1, \\ 1 & k = 2n, \\ 4n - 2k + 2 & 1 \leq k \leq 2n - 3 \text{ and } 2 \nmid k, \\ 5n - \frac{5}{2}k + 1 & 4 \leq k \leq 2n - 2 \text{ and } 2 \mid k, \end{cases}
$$

and

$$
d(\mathcal{O}_n, k) = \begin{cases} 4n & k = 1, \\ 6n - 4 & k = 2, \\ 8n - 12 & k = 3, \\ 15 & k = n, \\ 6 & k = n + 1, \\ 1 & k = n + 2, \\ 9n - 9k + 15 & 4 \leq k \leq n - 1. \end{cases}
$$

By applying the above relations and relation (2), one gets

$$RCW(\mathcal{Q}_n) = \sum_{k=1}^{D=2n} \frac{d(\mathcal{Q}_n, k)}{2n + 1 - k}$$

$$= 3 + \frac{6n - 4}{2n - 1} + \sum_{\substack{k=1 \\ 2 \nmid k}}^{2n-3} \frac{4n - 2k + 2}{2n - k + 1} + \sum_{\substack{k=4 \\ 2 \mid k}}^{2n-2} \frac{5n - \frac{5}{2}k + 1}{2n - k + 1}$$

$$= 2n + 1 + \frac{6n - 4}{2n - 1} + \sum_{k=2}^{n-1} \frac{5n - 5k + 1}{2n - 2k + 1} = \frac{18n^2 - 13n}{4n - 2} - \frac{3}{2} \sum_{k=1}^{n-2} \frac{1}{2k + 1},$$

as desired. The reciprocal complementary Wiener number of $\mathcal{O}_n$ can be computed by a similar way. $\square$

Theorem 2.3. *If $\mathcal{Q}_n$ ($n \geq 2$) is the Para-chain graph, then*

$$\frac{34n^3 - 75n^2 + 37n}{(4n - 2)(2n - 3)} \leq RCW(\mathcal{Q}_n) \leq \frac{18n^4 - 55n^3 + 77n^2 - 120n + 48}{2n(n - 2)(2n - 1)},$$

where each of the equalities holds if and only if $n = 3$.

Proof. If a_k and b_k are real numbers such that $a_k \neq 0$, and $m \leq \frac{b_k}{a_k} \leq M$, $k = 1, 2, \ldots l$, then

$$\sum_{k=1}^{l} b_k^2 + mM \sum_{k=1}^{l} a_k^2 \leq (M + m) \sum_{k=1}^{l} a_k b_k$$

with equality if and only if for all k, $1 \leq k \leq l$, either $b_k = ma_k$ or $b_k = Ma_k$. This inequality is known as the Diaz-Metcalf inequality. Considering $a_k^{-1} = b_k = \sqrt{2k + 1}$, $1 \leq k \leq n - 2$, in this inequality, we have

$$\sum_{k=1}^{n-2} \frac{1}{2k + 1} \leq \frac{n^2 - 2n}{3(2n - 3)}.$$

Using this inequality in part (i) of Theorem 2.2, the upper bound for $RCW(\mathcal{Q}_n)$ is obtained. We know from the Cauchy Schwartz inequality that if a_k and b_k are real numbers, $k = 1, 2, \ldots l$, then

$$\left(\sum_{k=1}^{l} a_k b_k \right)^2 \leq \left(\sum_{k=1}^{l} a_k^2 \right) \left(\sum_{k=1}^{l} b_k^2 \right)$$

where the equality holds if and only if $a_k = mb_k$ for a non-zero constant $m \in \mathbb{R}$. Now, considering $a_k^{-1} = b_k = \sqrt{2k + 1}$, $1 \leq k \leq n - 2$, in the Cauchy Schwartz inequality, we conclude that

$$\sum_{k=1}^{n-2} \frac{1}{2k + 1} \geq \frac{(n - 4)^2}{n^2 - 2n}.$$

Therefore, the lower bound for $RCW(\mathcal{Q}_n)$ is obtained by using this inequality in part (i) of Theorem 2.2. Finally, both equations occur when k is a constant value. This means that k must be 1 and n must be 3. □

Theorem 2.4. *If $\mathcal{O}_n$ ($n \geq 5$) is the Ortho-chain square cactus graph, then*

$$\frac{9n^5 - 3n^4 - 81n^3 + 113n^2 + 514n + 312}{n(n + 1)(n + 2)(n - 1)} \leq RCW(\mathcal{O}_n) \leq \frac{9n^5 + 21n^4 + 39n^3 + 41n^2 - 78n - 72}{n(n + 1)(n + 2)(n + 3)},$$

where each of the equalities holds if and only if $n = 5$.

Proof. Using similar arguments as in the proof of Theorem 2.3, if we consider $a_k^{-1} = b_k = \sqrt{k}$, $4 \leq k \leq n - 1$, in the Diaz-Metcalf and Cauchy Schwartz inequalities then we have

$$\frac{2(n - 4)^2}{n^2 - n - 12} \leq \sum_{k=4}^{n-1} \frac{1}{k} \leq \frac{n^2 - n - 12}{8(n - 1)}.$$

Therefore, bounds for $RCW(\mathcal{O}_n)$ is obtained by using this inequalities in part (ii) of Theorem 2.2. Also, both equations occur when $k = 4$. This means that n must be 5. □

Theorem 2.5. *Let $\mathcal{L}_n$ ($n \geq 3$) and $\mathcal{M}_n$ ($n \geq 4$) be the Para-chain and Meta-chain hexagonal cactus graphs, respectively. Then*

$$RCW(\mathcal{L}_n) = \frac{25}{3}n - 2 - \frac{4n - 2}{9n^2 - 9n + 2} - \frac{2}{3} \sum_{k=1}^{n-2} \frac{15k + 8}{9k^2 + 9k + 2} \quad \text{and}$$

$$RCW(\mathcal{M}_n) = \frac{25}{2}n + 11 - \frac{66n^3 + 55n^2 - 6n - 4}{4n^4 + 4n^3 - n^2 - n} - \sum_{k=1}^{n-1} \frac{35k - 8}{4k^2 - 2k}.$$

Proof. By [10], we have

$$
d(\mathcal{L}_n, k) = \begin{cases}
6n & k = 1, \\
10n - 4 & k = 2, \\
11n - 8 & k = 3, \\
8 & k = 3n - 2, \\
4 & k = 3n - 1, \\
1 & k = 3n, \\
8n - \frac{8k - 8}{3} & 4 \leq k \leq 3n - 5 \text{ and } k \equiv 1 \pmod 3, \\
8n - 4 - \frac{8k - 16}{3} & 5 \leq k \leq 3n - 4 \text{ and } k \equiv 2 \pmod 3, \\
9n - 3k + 1 & 6 \leq k \leq 3n - 3 \text{ and } 3 \mid k,
\end{cases}
$$

and

$$
d(\mathcal{M}_n, k) = \begin{cases}
6n & k = 1, \\
10n - 4 & k = 2, \\
11n - 8 & k = 3, \\
12n - 16 & k = 4, \\
16 & k = 2n - 1, \\
10 & k = 2n, \\
4 & k = 2n + 1, \\
1 & k = 2n + 2, \\
12n - 6k + 10 & 5 \leq k \leq 2n - 3 \text{ and } 2 \nmid k, \\
13n - \frac{13}{2}k + 10 & 6 \leq k \leq 2n - 2 \text{ and } 2 \mid k,
\end{cases}
$$

By applying the above relations and relation (2), one obtains

$$
RCW(\mathcal{L}_n) = \sum_{k=1}^{D=3n} \frac{d(\mathcal{L}_n, k)}{3n + 1 - k}
$$

$$
= \frac{23}{3} + \frac{10n - 4}{3n - 1} + \frac{11n - 8}{3n - 2} + \sum_{\substack{k=4 \\ k \equiv 1 \pmod 3}}^{3n-5} \frac{8n - \frac{8k - 8}{3}}{3n - k + 1}
$$

$$
+ \sum_{\substack{k=5 \\ k \equiv 2 \pmod 3}}^{3n-4} \frac{8n - 4 - \frac{8k - 16}{3}}{3n - k + 1} + \sum_{\substack{k=6 \\ 3 \mid k}}^{3n-3} \frac{9n - 3k + 1}{3n - k + 1}
$$

$$
= \frac{8}{3}n + \frac{28}{3} - \frac{4n - 2}{9n^2 - 9n + 2} + \sum_{k=1}^{n-2} \left(\frac{8n - 8k - 4}{3n - 3k - 1} + \frac{9n - 9k + 1}{3n - 3k + 1} \right)
$$

$$
= \frac{25}{3}n - 2 - \frac{4n - 2}{9n^2 - 9n + 2} - \frac{2}{3} \sum_{k=1}^{n-2} \frac{15k + 8}{9k^2 + 9k + 2},
$$

as desired. The reciprocal complementary Wiener number of $\mathcal{M}_n$ can be computed by a similar way. □

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