

## NEW VERSION OF SZEGED INDEX AND ITS COMPUTATION FOR SOME NANOTUBES

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The vertex and the first edge versions of Szeged index were introduced in last years. Very recently, A. Iranmanesh et al. introduced the second edge-Szeged index. In this paper, we introduce a new edge version for Szeged index and at following we compute this new index for some nanotubes.

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### 1. Introduction

A graph  $G$  consists of a set of vertices  $V(G)$  and a set of edges  $E(G)$ . In chemical graphs, each vertex presented an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph, and can be a path, a tree or in general a graph.

A topological index is a single number, derived following a certain rule which can be used to characterize the molecule [1]. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener [2] introduced Wiener number and the name of Wiener index was given by Hosoya [3].

Szeged index was introduced by Gutman and called the Szeged index, abbreviated as Sz [4]. The Szeged index is a modification of Wiener index to cyclic molecules. This was the vertex version of Sz index which had been defined as:

$$Sz_v(G) = \sum_{e=uv \in E(G)} n_e(u).n_e(v)$$

where  $n_e(u)$  is the number of vertices of  $G$  which are closer to  $u$  than  $v$  and  $n_e(v)$  is the number of vertices of  $G$  which are closer to  $v$  than  $u$ . In [5-11], you can find computations of this index for some graphs.

The edge version of Szeged index introduced recently by Gutman and Ashrafi that it is defined as [12]:

$$Sz_e(G) = \sum_{e=uv \in E(G)} m_e(u).m_e(v)$$

where  $m_e(u)$  is the number of edges of  $G$  which are closer to  $u$  than  $v$  and  $m_e(v)$  is the number of edges of  $G$  which are closer to  $v$  than  $u$ . We can restate  $m_e(u)$  and  $m_e(v)$  with mathematical notations as follow:

$m_e(u) = \left| \{f \in E(G) \mid d'(f,u) < d'(f,v)\} \right|$  and  $m_e(v) = \left| \{f \in E(G) \mid d'(f,v) < d'(f,u)\} \right|$  where  $d'$  is:

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If  $f = xy \in E(G)$  and  $u \in V(G)$ , then  $d'(f, u) = \min\{d(x, u), d(y, u)\}$ . In [13-14], this index was computed for some graphs.

The second edge-Szeged index is defined as follows:

$$Sz'_e(G) = \sum_{e=uv \in E(G)} m'_e(u) \cdot m'_e(v) \quad (1)$$

where  $m'_e(u) = |\{f \in E(G) \mid d''(f, u) < d''(f, v)\}|$  and  $m'_e(v) = |\{f \in E(G) \mid d''(f, v) < d''(f, u)\}|$ .

Also,  $d''$  is:

$$d''(f, u) = \begin{cases} d'(f, u) & u \text{ isn't in } f \\ 0 & u \text{ is in } f, \text{ (or } f = uv) \end{cases}$$

where if  $f = xy \in E(G)$  and  $u \in V(G)$ , then  $d''(f, u) = \max\{d(x, u), d(y, u)\}$ .

In this paper, we compute the second edge-Szeged index of well-known graphs and  $TUC_4C_8(S)$  nanotubes with usage the Matlab program (7.4.0 version).

## 2. Discussion and results

In this section, at first, we compute the second edge-Szeged index of several well-known graphs such as trees, cycles, complete graphs and bipartite complete graphs.

**Theorem 2-1.** The first edge-Szeged index is equal to the second-Szeged index for trees.

**Proof.** Let  $e = uv$  be an arbitrary edge in tree  $T$ . The tree  $T \setminus e$  contains two connected subtrees. One of them which contains the vertex  $u$  has  $n_e(u)$  vertices and  $m_e(u) = m'_e(u)$  edges that all of these edges are close to vertex  $u$  due to  $d'$  and  $d''$ . Another subtree which contains the vertex  $v$  has  $n_e(v)$  vertices and  $m_e(v) = m'_e(v)$  edges that all of these edges are close to vertex  $v$  due to  $d'$  and  $d''$ . Therefore,  $Sz_e(T) = Sz'_e(T)$ . ■

The first edge version of Szeged index of tree is:

$$Sz_e(T) = W(T) - W(S_n), \text{ where } S_n \text{ is the } n\text{-vertex star.}$$

Therefore, according to the Theorem (2-1), the second edge Szeged index of tree is:

$$Sz'_e(T) = W(T) - W(S_n)$$

For computing this index for some well known graphs, we state only the results that these results have come in table 1.

Table 1. The different versions of some well known graphs.

Graph $G$	$Sz_v(G)$	$Sz_e(G)$	$Sz'_e(G)$
$C_n, n$ is even	$\left(\frac{n}{2}\right)^2 n$	$\left(\frac{n-2}{2}\right)^2 n$	$\left(\frac{n-2}{2}\right)^2 n$
$C_n, n$ is odd	$\left(\frac{n-1}{2}\right)^2 n$	$\left(\frac{n-1}{2}\right)^2 n$	$\left(\frac{n-3}{2}\right)^2 n$
$K_n$	$\frac{1}{2}n(n-1)$	$\frac{1}{2}n(n-1)(n-2)^2$	$\frac{1}{2}n(n-1)(n-2)^2$
$K_{a,b}$ (Complete bipartite graphs)	$(ab)^2$	$ab(a-1)(b-1)$	$ab(a-1)(b-1)$

Due to the Table 1, we have for an especial case:

$$Sz'_e(K_{\lfloor \frac{n-1}{2} \rfloor, \lfloor \frac{n+1}{2} \rfloor}) = Sz_e(K_{\lfloor \frac{n-1}{2} \rfloor, \lfloor \frac{n+1}{2} \rfloor}) = \begin{cases} Sz'_e(K_{\frac{n}{2}, \frac{n}{2}}) = \frac{1}{16}n^2(n-2)^2 & , n = a + b \text{ is even} \\ Sz'_e(K_{\frac{n-1}{2}, \frac{n+1}{2}}) = \frac{1}{16}(n-3)(n-1)^2(n+1) & , n = a + b \text{ is odd} \end{cases}$$

Now, we state a conjecture. Before stating, we say a definition and prove a theorem which is as follows:

**Definition 2-2.** The edge  $f = xy$  is parallel to  $e = uv$  under  $d'$  (or  $d'''$ ) if  $d'(f, u) = d'(f, v)$  (or  $d'''(f, u) = d'''(f, v)$ ).

**Theorem 2-3.**  $Sz_e(G) \geq Sz'_e(G)$ , for arbitrary graph  $G$ .

**Proof.** Let  $G$  be an arbitrary graph. Then we have:

- I. If  $G$  is an acyclic graph. Then,  $Sz_e(G) = Sz'_e(G)$  due to the Theorem (2-1).
- II. If  $G$  is a cyclic graph. Then:
  - a) If  $G$  has an odd cycle, then  $Sz_e(G) \geq Sz'_e(G)$  due to Table 1.
  - b) If  $G$  has not odd cycle, select an edge  $e = uv$ .
    1. If  $e = uv$  is not in a cycle. Then,  $m_e(u) = m'_e(u)$  and  $m_e(v) = m'_e(v)$ . Because the graph  $G \setminus e$  has two component. In component which has vertex  $u$ , the edges of it is equal to  $m_e(u) = m'_e(u)$  that these edges are closer to  $u$  than  $v$ . Also, in another component which has vertex  $v$ , the edges of it is equal to  $m_e(v) = m'_e(v)$  that these edges are closer to  $v$  than  $u$ . Then for these edges which are not in cycle, we have:  $m_e(u)m_e(v) = m'_e(u)m'_e(v)$ .
    2. If  $e = uv$  is in a cycle. Then, we prove that the parallel edges with  $e$  under  $d'$  and  $d'''$  are equal together and therefore  $m_e(u)m_e(v) = m'_e(u)m'_e(v)$ . We denote this edges with two set  $A$  and  $B$  as follow:  $A = \{f \in E(G) \mid d'(f, u) = d'(f, v)\}$  and  $B = \{f \in E(G) \mid d'''(f, u) = d'''(f, v)\}$ . Therefore, it is enough that we show  $|A| = |B|$ . Let  $f \in A$ , then  $d'(f, u) = d'(f, v) \Rightarrow \min\{d(x, u), d(y, u)\} = \min\{d(x, v), d(y, v)\}$ . Then there are several subcases:
      - If  $d(x, v) = d(y, v) = d(x, u) = d(y, u)$ , then there exist at least an odd cycle which edge  $f$  is on this cycle and this case is a contradiction. For example, see Figure 1 (a).

- If  $d(x, v) = d(x, u) = d(y, u)$  are minimum distance, then there exist at least an odd cycle which edge  $f$  is on this cycle and this case is a contradiction. For example, see Figure 1 (a).
- If  $d(x, v) = d(x, u)$  are minimum distance, there exist at least an odd cycle which edge  $f$  is on this cycle and this case is a contradiction. For example, see Figure 1 (a).
- If  $d(x, u) = d(y, v)$  are minimum distance, due to the facts that cycles are even and Figure 1 (b),  $d(f, v) = d(x, v) = d(y, u) = d(f, u)$ . Because in other cases, we can find at least an odd cycle in graph  $G$ . Then  $A \subseteq B$ .

If  $f \in B$ , then  $d(f, u) = d(f, v) \Rightarrow \max\{d(x, u), d(y, u)\} = \max\{d(x, v), d(y, v)\}$ . Then there are several subcases:

- If  $d(x, v) = d(y, v) = d(x, u) = d(y, u)$ , then there exist at least an odd cycle which edge  $f$  is on this cycle and this case is a contradiction. For example, see Figure 1 (a).
- If  $d(x, v) = d(x, u) = d(y, u)$  are maximum distance, then there exist at least an odd cycle which edge  $f$  is on this cycle and this case is a contradiction. For example, see Figure 1 (a).
- If  $d(x, v) = d(x, u)$  are maximum distance, there exist at least an odd cycle which edge  $f$  is on this cycle and this case is a contradiction. For example, see Figure 1 (a).
- If  $d(x, u) = d(y, v)$  are maximum distance, due to the facts that cycles are even and Figure 1 (b),  $d(f, v) = d(x, v) = d(y, u) = d(f, u)$ . Because we can find at least an odd cycle in other cases. Then  $B \subseteq A$ .

Therefore  $A = B$  and  $|A| = |B|$ . Then  $m_e(u)m_e(v) = m'_e(u)m'_e(v)$ .

Hence  $Sz_e(G) = Sz'_e(G)$ , when  $G$  has no odd cycle.

Therefore,  $Sz_e(G) \geq Sz'_e(G)$ , for arbitrary graph  $G$ . ■

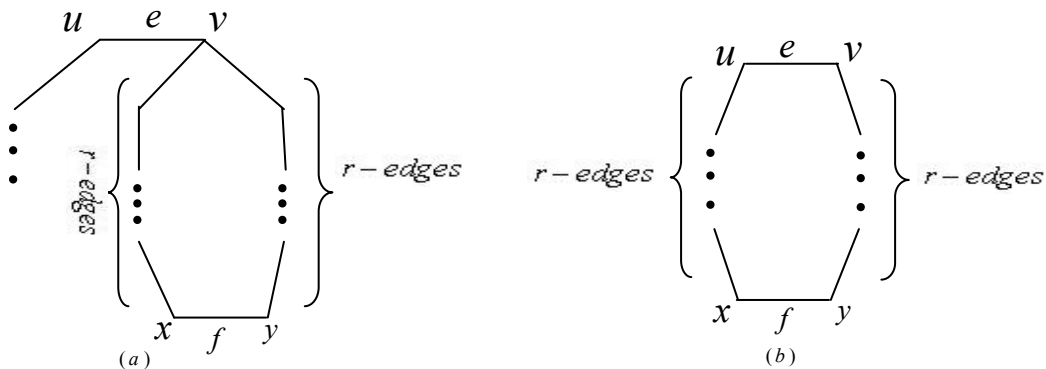


Fig. 1.

Therefore, due to Theorem (2-3), we state the conjecture about edge Szeged indices as follow:

**Conjecture.** The complete graph  $K_n$  has the greatest edge-Szeged indices among all  $n$ -vertex graphs.

In this section, we compute the second edge Szeged index of  $TUC_4C_8(S)$ . Due to the fact that there are not odd cycles in these graphs, we can obtain  $m_e(u)m_e(v) = m'_e(u)m'_e(v)$  for each edge (from proof of Theorem (2-3)). Therefore, we have  $Sz_e(G) = Sz'_e(G)$  for these graphs.

According to Figure 2, we denote the number of horizontal edges of squares in one row by  $p$  and the number of rows by  $k$ . Also, due to these notations,  $|E(G)| = 6pk - 2p$ .

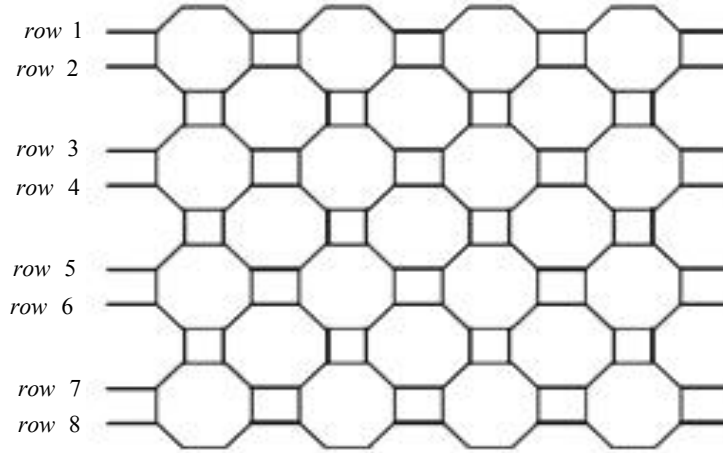


Fig. 2. Two dimensional lattice of  $TUC_4C_8(S)$  nanotube,  $p = 4, k = 8$ .

**Lemma 2-4.** Let  $e = uv$  be a horizontal edge in  $TUC_4C_8(S)$ , then:

$$m'_e(u) = m'_e(v) = \frac{(6pk - 2p - 2k)}{2} = 3kp - p - k.$$

**Proof.** It is easy to check according to Figure 2. ■

**Lemma 2-5.** Let  $e = uv$  be a vertical edge between  $m$  and  $(m+1)$  rows in  $TUC_4C_8(S)$ ,  $1 \leq m \leq k-1$ , then:

$$\begin{aligned} m'_e(u) &= 6pm - 2p \\ m'_e(v) &= 6pk - 6pm - 2p \end{aligned}$$

**Proof.** The desire results can be obtained easily according to Figure 2. ■

**Lemma 2-6.** Let  $e = uv$  be a oblique edge in  $m$ -th row in  $TUC_4C_8(S)$ ,  $1 \leq m \leq k$ , then:

$$m'_e(u) = \begin{cases} -2m - p + 3kp - k - k^2 + 4km & , m \leq p \ \& \ k - m \leq p \\ 3pm - 3m + 2m^2 - 2p + p^2 & , m \leq p \ \& \ k - m > p \\ -p^2 - 5p + 3mp + 3kp - k - 2k^2 + 4km - 2m^2 & , m > p \ \& \ k - m \leq p \\ 6mp - 6p - m & , m > p \ \& \ k - m > p \end{cases}$$

$$m'_e(v) = \begin{cases} 2m - p + 3kp - k + 2k^2 - 4km & , m \leq p \ \& \ k - m \leq p \\ -3mp + 2m - 2m^2 - p - p^2 + 6kp - k & , m \leq p \ \& \ k - m > p \\ p^2 + 3kp - k - 3mp + m + 2k^2 - 4km + 2m^2 & , m > p \ \& \ k - m \leq p \\ 6kp - 6mp - k + m & , m > p \ \& \ k - m > p \end{cases}$$

**Proof.** The desire results can be obtained easily according to Figure 2. ■

According to above results, the second edge-Szeged index of  $TUC_4C_8(S)$  nanotubes is stated in following theorem.

**Theorem2-7.** The second Szeged index of  $TUC_4C_8(S)$  is equal to:

$$Sz'_e(TUC_4C_8(S)) = \begin{cases} I & , k \leq p \\ II & , p < k \leq 2p \text{ , where I, II and III are:} \\ III & , k > 2p \end{cases}$$

$$I = -(2/3)k + (4/3)k^4 - 8p^3 - 30p^3k^2 + (2/3)k^2 + kp^2 + 21p^3k + 3k^3p^2 - 4k^2p^2 + 2k^2p - 5k^3p + 21p^3k^3 + k^3 - (4/3)k^5$$

$$II = (2/15)k + 18p^4k - (13/6)k^4 - p - 12p^5 - 33p^3 + 32p^4 - 30p^3k^2 - (17/3)kp + (2/3)k^2 + 8p^2 + (161/6)kp^2 - 24p^3k - (28/3)k^3p^2 + (15/2)k^2p^2 - (1/2)k^2p + 5k^4p + (13/6)k^3p + 21p^3k^3 - (5/6)k^3 - (4/5)k^5$$

$$III = -(1/6)k - (2/5)p + (1/3)kp + (17/3)p^2 - 16k^2p^2 + 3k^2p + 2kp^4 - (4/15)p^5 - k^3p + (224/3)p^3k - 30p^3k^2 + (1/6)k^3 - 5kp^2 + 21p^3k^3 - (134/3)p^4 - (118/3)p^3$$

**Proof.** With applying the Lemmas (2-4, 2-5 and 2-6) and due to the fact that there are  $2p$  horizontal edges in a row,  $2p$  vertical edges between rows and  $2p$  oblique edges in a row, we sum the  $2p(m'_e(u)m'_e(v))$  for each type of edges for all rows. Then with using the Matlab program (7.4.0 version), the desire results can be found. ■

### 3. Conclusion

At follows, the second edge Szeged index of  $TUC_4C_8(R)$  is computed.

According to Figure 3,  $k$  is the number of rows of rhombus and  $p$  is the number of rhombus in a row (that  $p$  indicates the number of columns of rhombus in Figure 3). Therefore, we can indicate the rhombus which located in  $i$  – th row and  $j$  – th column with  $S_{ij}$ . Also,  $|V(G)| = 4pk$  and  $|E(G)| = 6pk - p$ .

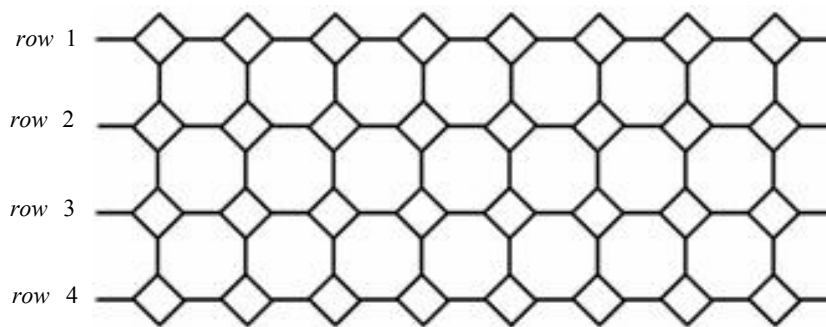


Fig. 3. Two dimensional lattice of  $TUC_4C_8(R)$  nanotube,  $k = 4, p = 8$ .

**Lemma 3-1.** Let  $e = uv$  be a horizontal edge in  $TUC_4C_8(R)$ , then:

$$m'_e(u) = m'_e(v) = \begin{cases} 3kp - \frac{p}{2} - k & , \text{if } p \text{ is even} \\ 3kp - \frac{p}{2} - k - \frac{1}{2} & , \text{if } p \text{ is odd} \end{cases}$$

**Proof.** It is easy to check according to Figure 3. ■

**Lemma 3-2.** Let  $e = uv$  be a vertical edge between  $m$  and  $(m+1)$  rows in  $TUC_4C_8(R)$ ,  $1 \leq m \leq k-1$ , then:

$$\begin{aligned} m'_e(u) &= 6pm - p \\ m'_e(v) &= 6pk - 6pm - p \end{aligned}$$

**Proof.** The desired results can be obtained easily according to Figure 3. ■

**Lemma 3-3.** Let  $e = uv$  be an oblique edge in  $m$ -th row in  $TUC_4C_8(R)$ ,  $1 \leq m \leq k$ , then:

1. If  $p$  is even:

$$m'_e(u) = \begin{cases} 3kp - 4k - 3k^2 + 6km & , m \leq \frac{p}{2} \text{ \& } k - m \leq \frac{p}{2} \\ 3mp - 4m + 3m^2 + \frac{3}{4}p^2 - 2p & , m \leq \frac{p}{2} \text{ \& } k - m > \frac{p}{2} \\ 1 - 4k + 3m - \frac{5}{2}p + 3mp - 3m^2 + \\ \quad 3kp - 3k^2 + 6km - \frac{3}{4}p^2 & , m > \frac{p}{2} \text{ \& } k - m \leq \frac{p}{2} \\ -\frac{9}{2}p + 6mp - m + 1 & , m > \frac{p}{2} \text{ \& } k - m > \frac{p}{2} \end{cases}$$

$$m'_e(v) = \begin{cases} 3kp + k + 3k^2 - 6km & , m \leq \frac{p}{2} \text{ \& } k - m \leq \frac{p}{2} \\ -3mp + 2m - 3m^2 - \frac{3}{4}p^2 + p + 6kp - k & , m \leq \frac{p}{2} \text{ \& } k - m > \frac{p}{2} \\ \frac{3}{4}p^2 + \frac{p}{2} + 3kp + k - 3mp - m + 3k^2 - 6km + 3m^2 & , m > \frac{p}{2} \text{ \& } k - m \leq \frac{p}{2} \\ \frac{3}{2}p + 6kp - 6mp - k + m & , m > \frac{p}{2} \text{ \& } k - m > \frac{p}{2} \end{cases}$$

2. If  $p$  is odd:

$$m'_e(u) = \begin{cases} -m \left\lfloor \frac{p}{2} \right\rfloor - m + m \left\lfloor \frac{p}{2} \right\rfloor + 6k \left\lfloor \frac{p}{2} \right\rfloor - k - 3k^2 + 6km & , m \leq \left\lfloor \frac{p}{2} \right\rfloor \& k - m \leq \left\lfloor \frac{p}{2} \right\rfloor \\ 5m \left\lfloor \frac{p}{2} \right\rfloor - 2m + 3m^2 + m \left\lfloor \frac{p}{2} \right\rfloor + 3 \left\lfloor \frac{p}{2} \right\rfloor^2 - \left\lfloor \frac{p}{2} \right\rfloor & , m \leq \left\lfloor \frac{p}{2} \right\rfloor \& k - m > \left\lfloor \frac{p}{2} \right\rfloor \\ 5 \left\lfloor \frac{p}{2} \right\rfloor \left\lfloor \frac{p}{2} \right\rfloor - 2 \left\lfloor \frac{p}{2} \right\rfloor + 4 \left\lfloor \frac{p}{2} \right\rfloor^2 + 6pm - 6p \left\lfloor \frac{p}{2} \right\rfloor - & , m > \left\lfloor \frac{p}{2} \right\rfloor \& k - m \leq \left\lfloor \frac{p}{2} \right\rfloor \\ p + 6k \left\lfloor \frac{p}{2} \right\rfloor - k - 6m \left\lfloor \frac{p}{2} \right\rfloor + m - 3k^2 + 6km - 3m^2 & \\ 5 \left\lfloor \frac{p}{2} \right\rfloor \left\lfloor \frac{p}{2} \right\rfloor - 2 \left\lfloor \frac{p}{2} \right\rfloor + 4 \left\lfloor \frac{p}{2} \right\rfloor^2 + 6pm - 6p \left\lfloor \frac{p}{2} \right\rfloor - & , m > \left\lfloor \frac{p}{2} \right\rfloor \& k - m > \left\lfloor \frac{p}{2} \right\rfloor \\ p + 3 \left\lfloor \frac{p}{2} \right\rfloor^2 - \left\lfloor \frac{p}{2} \right\rfloor & \end{cases}$$

$$m'_e(v) = \begin{cases} m \left\lfloor \frac{p}{2} \right\rfloor + m - m \left\lfloor \frac{p}{2} \right\rfloor + 5k \left\lfloor \frac{p}{2} \right\rfloor + 4k + 3k^2 - 6km + k \left\lfloor \frac{p}{2} \right\rfloor & , m \leq \left\lfloor \frac{p}{2} \right\rfloor \& k - m \leq \left\lfloor \frac{p}{2} \right\rfloor \\ 6m \left\lfloor \frac{p}{2} \right\rfloor - pm + pk - 3m^2 + 8 \left\lfloor \frac{p}{2} \right\rfloor^2 - \left\lfloor \frac{p}{2} \right\rfloor + \left\lfloor \frac{p}{2} \right\rfloor \left\lfloor \frac{p}{2} \right\rfloor + & \\ 5k - p \left\lfloor \frac{p}{2} \right\rfloor & , m \leq \left\lfloor \frac{p}{2} \right\rfloor \& k - m > \left\lfloor \frac{p}{2} \right\rfloor \\ 6 \left\lfloor \frac{p}{2} \right\rfloor \left\lfloor \frac{p}{2} \right\rfloor + 5 \left\lfloor \frac{p}{2} \right\rfloor - 3 \left\lfloor \frac{p}{2} \right\rfloor^2 - m \left\lfloor \frac{p}{2} \right\rfloor + k \left\lfloor \frac{p}{2} \right\rfloor + 5k \left\lfloor \frac{p}{2} \right\rfloor + & , m > \left\lfloor \frac{p}{2} \right\rfloor \& k - m \leq \left\lfloor \frac{p}{2} \right\rfloor \\ 4k - 5m \left\lfloor \frac{p}{2} \right\rfloor - 4m + 3k^2 - 6km + 3m^2 & \\ 4 \left\lfloor \frac{p}{2} \right\rfloor \left\lfloor \frac{p}{2} \right\rfloor + 2 \left\lfloor \frac{p}{2} \right\rfloor + 8 \left\lfloor \frac{p}{2} \right\rfloor^2 + 5k - 5m + pk - pm - & \\ p \left\lfloor \frac{p}{2} \right\rfloor - \left\lfloor \frac{p}{2} \right\rfloor & , m > \left\lfloor \frac{p}{2} \right\rfloor \& k - m > \left\lfloor \frac{p}{2} \right\rfloor \end{cases}$$

**Proof.** The desired results can be obtained easily according to Figure 3. ■

**Theorem 3-4.** The second Szeged index of  $TUC_4C_8(R)$  is equal to:

1. If  $p$  is even:



$$Sz'_e(TUC_4C_8(R)) = \begin{cases} I & , k \leq \frac{p}{2} \\ II & , \frac{p}{2} < k \leq p \text{ , where I, II and III are:} \\ III & , k > p \end{cases}$$

$$I = -6p^3k^2 - pk^2 + 3k^2p^2 + 10k^3p - p^3 + 24p^3k^3 + p^3k - 18k^3p^2 - 6pk^5 - (1/2)kp^2$$

$$II = -39p^4k + 9kp^5 + (289/16)p^5 + 17p^3 - (377/12)p^4(-27/8)p^6 - 2/5kp - (5/6)p^2 - 7kp^2 + (185/4)p^3k + 6p^3k^3 - 6p^3k^2 - 14k^2p + 17k^2p^2 - 22k^3p + 12k^4p^2 + 22k^3p^2 - 17pk^4 - (18/5)k^5p$$

$$III = 7p^4k - (15/16)p^5 + p^3 + (9/4)p^4 - 24p^3k^2 + (2/3)kp - (19/10)p^2 - 3kp^2 - (19/4)p^3k - 4k^3p^2 + 12k^2p^2 - 2k^2p + (1/3)k^3p + 3p^5k + 18p^3k^3 - (39/40)p^6$$

2. If  $p$  is odd:

$$Sz'_e(TUC_4C_8(R)) = \begin{cases} I & , k \leq \left\lfloor \frac{p}{2} \right\rfloor \\ II & , \left\lfloor \frac{p}{2} \right\rfloor < k \leq p \text{ , where I, II and III are:} \\ III & , k > p \end{cases}$$

$$I = -5/6kp + 2p[(1/2)p] + 1)k^2 + 2/3pk(1/2)p[(1/2)p] + 1) + 34/3pk^3(1/2)p[(1/2)p] + 1) + p^3k + 6p^3k^3 - 6p^3k^2 - p^3 - 1/3p[(1/2)p] + 1)k - 1/3p((1/2)p)^2k - 2/3p(1/2)pk + 2/3[(1/2)p] + 1)k + 1/3p[(1/2)p] + 1)^2k^3 + 181/3p((1/2)p)^2k^3 + 2pk^4(1/2)p - 2pk^4[(1/2)p] + 1) - 6pk^5 + 3k^2p^2 - 1/2kp^2 - 2pk^2(1/2)p - 3pk^2 + 31/3pk^3 + 2pk^4 + 98/3pk^3(1/2)p + 10/3pk^3[(1/2)p] + 1)$$

$$II = -10p^2[(1/2)p] + 1)k^3 - 6p^2k[(1/2)p] + 30pk((1/2)p)^2 - (23/2)p[(1/2)p] + 1)((1/2)p)^2 + (4/3)pk[(1/2)p] - (37/30)kp + p[(1/2)p]^2 - (25/2)k^2p + 6p^3k^3 - 42p^2[(1/2)p] + 1)^2k[(1/2)p] + p^3k + (11/15)[(1/2)p] + 1)p - (33/2)pk^4 + (3/5)p[(1/2)p] + 35p^2[(1/2)p] + 1)k[(1/2)p] - p^3 - 6p^3k^2 + 43p[(1/2)p]^4 - (38/3)p^2[(1/2)p]^3 - (37/2)[((1/2)p)]^3p + 14p[[(1/2)p]]^3[(1/2)p] + 1) + 4p^2[[(1/2)p]]^2k + (5/6)p^2[[(1/2)p]]^2 + 6p^2k^3 - (71/3)k^3p - (18/5)pk^5 + 3p^2k^4 - p^2k^2 - (11/2)p^2k + (8/3)p[(1/2)p] + 1)k + 6p[(1/2)p] + 1)^2k - 16pk^3[(1/2)p] + 1)^2 + (1339/10)p[[(1/2)p]]^5 + (2/3)p^2[(1/2)p] + (211/6)p[(1/2)p] + 1)^3 - (67/6)p[(1/2)p] + 1)^2 + (161/10)p[(1/2)p] + 1)^5 - (245/6)p[(1/2)p] + 1)^4 - 23p^2[(1/2)p] + 1)^2 + 5p^2[(1/2)p] + 1) - (125/6)p^2[[(1/2)p]]^4 - 17p^2[[(1/2)p]]^4 + 35p^2[(1/2)p] + 1)^3 + 4p[(1/2)p] + 1)^3[(1/2)p]k - p[(1/2)p] + 1)[(1/2)p]k + 6p[(1/2)p] + 1)^2[(1/2)p]k - 10p[(1/2)p] + 1)[(1/2)p]k^2 + 6pk[[(1/2)p]]^2[(1/2)p] + 1) - 2pk[[(1/2)p]]^2[(1/2)p] + 1)^2 + 10p[(1/2)p] + 1)^2[(1/2)p]k^2 + pk^2[[(1/2)p]]^2[(1/2)p] + 1) - 4p[(1/2)p] + 1)[(1/2)p]k^3 + 6p^2[(1/2)p] + 1)k^2[(1/2)p] + p^2(1/2)pk[(1/2)p] + 1)^2 - (23/2)[(1/2)p] + 1)^4p[(1/2)p] + (19/3)[(1/2)p] + 1)^3p[(1/2)p] - (19/3)[(1/2)p] + 1)p[(1/2)p] + (23/2)[(1/2)p] + 1)^2p[(1/2)p] - 52p^2[(1/2)p] + 1)^2k + (145/3)pk^3[(1/2)p] + 1) + (3/2)p[(1/2)p]k^4 + (47/3)p[(1/2)p]k^3 + (41/2)p[(1/2)p]k^2 + 30p^2[(1/2)p] + 1)^3k - 19p[(1/2)p] + 1)^3[(1/2)p]^2 + 65kp[(1/2)p]^3 - 29p^2[(1/2)p] + 1)^2[(1/2)p] + 26p^2[(1/2)p] + 1)^3[(1/2)p] - (5/3)p^2[(1/2)p] + 1)[(1/2)p]^3 - 2p^2[(1/2)p] + 1)[(1/2)p]^2 - 2p[(1/2)p] + 1)^4k - 7p[(1/2)p] + 1)^3k + (33/2)pk^4[(1/2)p] + 1) +$$

$$13p^2k[(1/2)p]^3 - 6p^2[(1/2)p+1]^2k^2 + 30p[(1/2)p+1]^2[(1/2)p]^2 + 27p^2[(1/2)p+1]k + (14/3)p^2[(1/2)p+1][(1/2)p] + 30pk^2[(1/2)p]^2 + 11p^2[(1/2)p+1]k^2 + (69/2)p[(1/2)p+1]k^2 - 8p[(1/2)p+1]^2k^2 + (47/2)[(1/2)p+1]p[(1/2)p]^4 + [(1/2)p+1]^2p[(1/2)p]^3 - 11p[(1/2)p+1]^3k^2 + 10p^2[(1/2)p]k^3 - 5p^2[(1/2)p]k^2 + 20p[(1/2)p]^2k^3$$

$$\begin{aligned} III = & -76[(1/2)p+1]kp^2[(1/2)p]^2 - (1/2)kp - (13/6)p[(1/2)p]^2 - k^2p - 63p[(1/2)p+1]^2[(1/2)p]^3 + 104p[(1/2)p+1] \\ & [(1/2)p]^3k - 60p^2[(1/2)p]^3k + (3/5)[(1/2)p+1]p - (1/3)[(1/2)p+1]p^2 - (301/10)p[(1/2)p]^5 - 29p[(1/2)p+1]^4 + \\ & (105/2)p[(1/2)p+1]^3 + p^3[(1/2)p+1] - 2p^3[(1/2)p+1]^3 - p^3[(1/2)p+1]^2 - p^3[(1/2)p]^2 + (11/6) \\ & [(1/2)p+1]^4p^2 + p^3[(1/2)p] - 2p^3[(1/2)p]^3 + 22p^2[(1/2)p]^4 - 19p[(1/2)p+1]^2 - \\ & (51/10)p[(1/2)p+1]^5 + (11/15)p[(1/2)p] + 8p^3k^3 + 10p^2k^3 - p^3 - \\ & (269/6)p^2[(1/2)p+1]^2 + 43[(1/2)p+1]p^2[(1/2)p]^3 + 4p^2[(1/2)p+1]^2k^2 + 51p^2k^2[(1/2)p]^2 - (125/3) \\ & [(1/2)p+1]p^2[(1/2)p] - 6p^3k^2[(1/2)p] + 6p^3k[(1/2)p]^2 - 5p[(1/2)p]k^2 + \\ & 15pk^2[(1/2)p]^2 - (11/2)kp^2 - 2p^2k^2 - 7p^3k^2 + 98[(1/2)p+1]p^2[(1/2)p]k + 55[(1/2)p+1]kp^2 - \\ & (71/6)p[(1/2)p]^4 + 9p^2[(1/2)p]^3 - 13p^2[(1/2)p]^2 + 9101/6[(1/2)p]^3p + \\ & (142/3)p[(1/2)p]^3[(1/2)p+1] + (49/2)p[(1/2)p+1][(1/2)p]^2 - 11p^2[(1/2)p]^2k + 9p^2[(1/2)p]k + 5pk[(1/2)p] - \\ & 13pk[(1/2)p]^2 + (112/3)p^2[(1/2)p+1]^3 - 6p^3[(1/2)p+1]k^2 - \\ & 28p^2[(1/2)p+1]^2k + 57p[(1/2)p+1]^3[(1/2)p] + 2p[(1/2)p+1]^2k - (52/3)p[(1/2)p+1] \\ & [(1/2)p] + 5p[(1/2)p+1]k + 2p^3[(1/2)p+1]k - 2p^3[(1/2)p+1][(1/2)p] - 33p^2[(1/2)p+1] \\ & [(1/2)p]^2 + 93p[(1/2)p+1]^2[(1/2)p]^2 - 10p[(1/2)p+1]k^2 - (95/2)p[(1/2)p+1]^4[(1/2)p] - 5p^2[(1/2)p+1]^3k - \\ & 9p[(1/2)p+1]^3k + (67/2)p[(1/2)p+1]^2[(1/2)p] + \\ & 45p^2[(1/2)p+1]^2[(1/2)p]^2 - 6p^3[(1/2)p+1]^2[(1/2)p] + 6p^3[(1/2)p+1]^2k - \\ & 71p[(1/2)p+1][(1/2)p]^2 + 48p[(1/2)p]^4k + 2p^3k[(1/2)p] + (200/3)[(1/2)p+1]^3p^2[(1/2)p] + 20p[(1/2)p+1]^2k^2 - \\ & 66[(1/2)p+1]^2p^2[(1/2)p] - (85/2)p[(1/2)p+1][(1/2)p]^4 - 7p^2[(1/2)p]k^2 - 20[(1/2)p+1]k^2p^2 - 6p^3[(1/2)p+1] \\ & [(1/2)p]^2 + 29[(1/2)p+1]p^2[(1/2)p]k^2 + 25pk^2[(1/2)p] \\ & [(1/2)p+1] + 12p^3[(1/2)p+1]k[(1/2)p] + 32p[(1/2)p+1]^3k[(1/2)p] - 38p[(1/2)p+1][(1/2)p]^2k - 29pk[(1/2)p] \\ & [(1/2)p+1]^2 + 104p[(1/2)p+1]^2[(1/2)p]^2k - 97[(1/2)p+1]^2p^2[(1/2)p]k - 22pk[(1/2)p]^3 \end{aligned}$$

**Proof.** With applying the Lemmas (3-1, 3-2 and 3-3) and due to the fact that there are  $p$  horizontal edges in a row,  $p$  vertical edges between rows and  $2p$  oblique edges in a row, we sum the  $(m'_e(u)m'_e(v))$  for each edge of the different types of edges for all rows according to  $p$  is odd or even. Then with using the Matlab program (7.4.0 version), the desire results can be found. ■

## References

- [1] I. Gutman, Y. N. Yeh, S. L. Lee and Y. L. Luo, J. Chem. **32A**, 651 (1993).
- [2] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc., **69**, 17 (1947).
- [3] H. Hosoya, Bull. Chem. Soc. Jap. **44**, 2322 (1971).
- [4] I. Gutman, Graph theory notes, New York, **27**, 1994.
- [5] A. Iranmanesh, O. Khormali, J. Comput. Theor. Nanosci., in press.
- [6] A. Iranmanesh, Y. Pakraves, Journal of applied sciences, **7**(23), 3606 (2007).
- [7] A. Iranmanesh B. Soleimani, A. Ahmadi, J. Comput. Theor. Nanosci, **4**(1), 147 (2007).
- [8] A. Iranmanesh, Y. Pakraves, Utilitas Mathematica, **75**, 89 (2008).
- [9] A. Iranmanesh, Y. Pakraves, A. Mahmiani, Ars Combinatorics, **87**, 193 (2008).
- [10] A. Iranmanesh, N. Gholami, Croatica Chemica Acta, **81**, 299 (2008).
- [11] A. Iranmanesh, Y. Alizadeh, Digest Journal of Nanomaterials and Biostructures, **4**, (1), 67 (2009).
- [12] I. Gutman, A. R. Ashrafi, Croat. Chem. Acta, **81**(2), 263 (2008).
- [13] D. Vukicevic, Math. Comput. Chem., **61**(3), 673 (2009).
- [14] A. Iranmanesh, Y. Pakraves, A. Mahmiani, Utilitas Mathematica, **77**, 65 (2008).