

Relations among the edge detour polynomials in nanotubes

SH. SAFARI SABET^a, M. FARMANI^a, O. KHORMALI^{b,*}, A. MAHMIANI^c AND Z. BAGHERI^d

^aDepartment of Mathematics, Islamic Azad University Central Tehran branch, Tehran, Iran

Email: drsafarisabet@gmail.com

Email: mino.farmani@yahoo.com

^bMathematics and Informatics Research Group, ACECR, Tarbiat Modares University

P.O.Box: 14115-343, Tehran, Iran

Email: o_khormali@modares.ac.ir

^cDepartment of Mathematics, Payame Noor University, 19395-4797, Tehran, Iran

Email: mahmiani@pnu.ac.ir

^dIslamic Azad University Branch of Azadshaher, Azadshaher, Iran

Email: bagheri@yahoo.com

ABSTRACT. The edge detour polynomials were recently introduced for computing the edge detour indices. In this paper, we find relations among edge detour polynomials and then, edge detour indices, by using graph theoretical techniques in molecular graphs. These relations are computed for the nanotubes $TUC_4C_8(S)$, $TUC_4C_8(R)$ and armchair polyhex nanotubes.

Keywords: Detour index, Edge detour indices, Edge detour polynomials, Line graph, Nanotube.

1. INTRODUCTION

The structure of a chemical compound is usually modeled by using molecular graphs. It has been found that many properties of a chemical compound are closely related

*Corresponding author

with some topological indices of its molecular graph. A graph $G = (V, E)$ is a combinatorial object consisting of an arbitrary set $V = V(G)$ of vertices and a set $E = E(G)$ of unordered pairs $(x, y) = xy$ of distinct vertices of G called edges. In a molecular graph, vertices are atoms while the edges represent covalent bonds.

Among the topological indices, the Wiener number is the oldest and probably the most important one [1]. The Wiener index, a distance-based invariant, was introduced by H. Wiener about 60 years ago to demonstrate correlations between the thermodynamic properties of alkanes and their molecular graphs. Topological indices have found applications in communication, facility location, cryptology, etc. [2].

The detour index was introduced in graph theory some time ago by F. Harary in describing the connectivity in directed graphs [3]. The detour index, in contrast to the Wiener index (that counts the length of the shortest path between pair vertices), considers the length of the longest path between each pair of vertices. This index has recently received some attention in the chemical literature [4,5]. The detour index certainly carries some interesting structural information for cyclic compounds. For acyclic structures the Wiener index and the detour index are the same, since there is only a single possible path connecting any pair of vertices [1]. The detour index is defined as follows:

$$D(G) = \sum_{\{u,v\} \subseteq V(G)} \Delta(u,v) \quad (1)$$

where $\Delta(u,v)$ denotes the detour between the vertices u and v (i.e. the number of edges on the longest path joining them).

The detour polynomial of graph G was introduced recently [6]. The detour polynomial of G is

$$D(G; x) = \sum_{\{x,y\} \subseteq V(G)} x^{\Delta(x,y)} \quad (2)$$

Also, the edge versions of detour index are the sum of distances between edges of a connected graph G on the longest path as follow [7]:

the first edge-detour index is:

$$D_{e0}(G) = \sum_{\{e,f\} \in E(G)} \Delta_0(e,f) = \sum_{\{e,f\} \in V(L(G))} \Delta_0(e,f) \quad (3)$$

where $\Delta_0(u,v)$ is the detour index in the line graph (also called the edge intersection graph) $L(G)$, where vertices correspond to edges of G and vertices in $L(G)$ are adjacent if the corresponding edges share an angle.

The second edge-detour index is:

$$D_{e3}(G) = \sum_{\{e,f\} \in E(G)} \Delta_3(e,f) \quad (4)$$

where $\Delta_3(e,f) = \begin{cases} \Delta_1(e,f) + 1 & , e \neq f \\ 0 & , e = f \end{cases}$ and $\Delta_1(e,f) = \min\{\Delta(u,x), \Delta(u,y), \Delta(v,x), \Delta(v,y)\}$ where $e = uv$ and $f = xy$.

The third edge-detour index is:

$$D_{e4}(G) = \sum_{\{e,f\} \in E(G)} \Delta_4(e,f) \quad (5)$$

where $\Delta_4(e, f) = \begin{cases} \Delta_2(e, f) & , e \neq f \\ 0 & , e = f \end{cases}$ and $\Delta_2(e, f) = \max\{\Delta(u, x), \Delta(u, y), \Delta(v, x), \Delta(v, y)\}$ where $e = uv$ and $f = xy$.

In addition, the edge detour polynomials are introduced recently as follows [8]:

$$D_{e_i}(G; x) = \sum_{\{e, f\} \in E(G)} x^{\Delta_i(e, f)} \text{ where } i = 0, 3, 4. \quad (6)$$

Finding the relations among edge detour polynomials and also edge detour indices are not reported so far. Therefore, due to the applications of nanostructures in particular nanotubes [9, 10 and 11] and edge detour polynomials, introduced recently by the authors, we present here the complete mentioned relations. As examples, we calculate these relations for some nanotubes, $TUC_4C_8(S)$, $TUC_4C_8(R)$ and armchair polyhex nanotubes.

2. RESULT AND DISCUSSION

In view of drawing our results, let first restate the edge detour polynomials according to topological distances in G and $L(G)$ [8].

Definition 1. Let $e, f \in E(G)$, $e = uv$ and $f = xy$. Fix a longest path between edges e and f and name it P . We define the quantity $\Delta'_p(e, f)$ as follows [8]:

$$\Delta'_p(e, f) = \min\{\Delta_p(u, x), \Delta_p(u, y), \Delta_p(v, x), \Delta_p(v, y)\}$$

where Δ_p is length of the path P . If the edge detour is defined as the longest path between edges, we can imagine six cases (Figure 1).

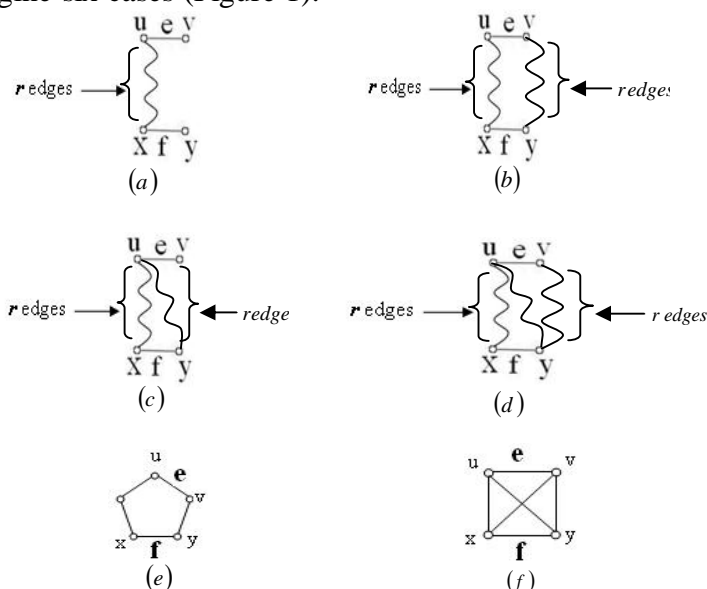


Figure 1. The quantity $\Delta'_p(e, f)$ is r for shapes (a,b,c and d) and is 1 for shapes (e and f).

Therefore, we partition the set of pair edges into the following subsets.

$$A_1 = \{\{e, f\} \subseteq E(G) \mid e, f, \text{Figure 1(a)}\}; A_2 = \{\{e, f\} \subseteq E(G) \mid e, f, \text{Figure 1(b)}\};$$

$$A_3 = \{\{e, f\} \subseteq E(G) \mid e, f, \text{Figure 1(c)}\}; A_4 = \{\{e, f\} \subseteq E(G) \mid e, f, \text{Figure 1(d)}\};$$

$$A_5 = \{\{e, f\} \subseteq E(G) \mid e, f, \text{Figure 1}(e)\}; A_6 = \{\{e, f\} \subseteq E(G) \mid e, f, 1(f)\}$$

Then, we find the edge detours as follows:

Lemma 2. Let $e, f \in E(G)$, $e = uv$ and $f = xy$. Then [8],

$$\Delta_0(e, f) = \begin{cases} \Delta'(e, f) + 1, & \{e, f\} \in A_1 \\ \Delta'(e, f) + 1, & \{e, f\} \in A_2 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_3 \\ 3\Delta'(e, f) + 1, & \{e, f\} \in A_4 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_5 \\ 4\Delta'(e, f) + 1, & \{e, f\} \in A_6 \end{cases}, \Delta_3(e, f) = \begin{cases} \Delta'(e, f) + 1, & \{e, f\} \in A_1 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_2 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_3 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_4 \\ \Delta'(e, f) + 3, & \{e, f\} \in A_5 \\ 3\Delta'(e, f) + 1, & \{e, f\} \in A_6 \end{cases} \text{ and}$$

$$\Delta_4(e, f) = \begin{cases} \Delta'(e, f) + 2, & \{e, f\} \in A_1 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_2 \\ \Delta'(e, f) + 2, & \{e, f\} \in A_3 \\ 3\Delta'(e, f), & \{e, f\} \in A_4 \\ \Delta'(e, f) + 3, & \{e, f\} \in A_5 \\ 3\Delta'(e, f), & \{e, f\} \in A_6 \end{cases}$$

Theorem 3. The relations between edge-detour index polynomials are [8]:

$$D_{e_0}(G; x) - D_{e_3}(G; x) = (1-x) \sum_{\{e, f\} \in A_2} x^{(\Delta'(e, f)+1)} + \sum_{\{e, f\} \in A_4} x^{(\Delta'(e, f)+2)} (x^{(2\Delta'(e, f)-1)} - 1) \\ + (1-x) \sum_{\{e, f\} \in A_5} x^{(\Delta'(e, f)+2)} + \sum_{\{e, f\} \in A_6} x^{(3\Delta'(e, f)+1)} (x^{\Delta'(e, f)} - 1). \quad (7)$$

and

$$D_{e_0}(G; x) - D_{e_4}(G; x) = (1-x) \sum_{\{e, f\} \in A_1} x^{(\Delta'(e, f)+1)} + (1-x) \sum_{\{e, f\} \in A_2} x^{(\Delta'(e, f)+1)} \\ + (x-1) \sum_{\{e, f\} \in A_4} x^{(3\Delta'(e, f))} + (1-x) \sum_{\{e, f\} \in A_5} x^{(\Delta'(e, f)+2)} \\ + \sum_{\{e, f\} \in A_6} x^{(3\Delta'(e, f))} (x^{(\Delta'(e, f)+1)} - 1) \quad (8)$$

Result 4. The relations between edge detour indices are [8]:

$$D_{e_0}(G) - D_{e_3}(G) = 2 \sum_{\{e, f\} \in A_4} \Delta'(e, f) + \sum_{\{e, f\} \in A_6} \Delta'(e, f) - |A_2| - |A_4| - |A_5| \quad (9)$$

and

$$D_{e_0}(G) - D_{e_4}(G) = \sum_{\{e, f\} \in A_6} \Delta'(e, f) - |A_1| - |A_2| + |A_4| - |A_5| + |A_6|. \quad (10)$$

In the following, we draw the relation between edge detour polynomials $D_{e_3}(G; x)$ and $D_{e_4}(G; x)$; also, we find the relation between edge detour indices $D_{e_3}(G)$ and $D_{e_4}(G)$.

Result 5. The relations between edge detour polynomials $D_{e_3}(G; x)$ and $D_{e_4}(G; x)$ are:

$$D_{e_4}(G; x) - D_{e_3}(G; x) = -(1-x) \sum_{\{e,f\} \in A_4} x^{(\Delta'(e,f)+1)} + \sum_{\{e,f\} \in A_4} x^{\Delta'(e,f)} (x^{2\Delta'(e,f)} - x^2) + \sum_{\{e,f\} \in A_6} x^{3\Delta'(e,f)} (1-x) \quad (11)$$

Proof. By using the Eqs 9 and 10, and replacing then in $D_{e_4}(G; x) - D_{e_3}(G; x)$, we have

$$\begin{aligned} D_{e_4}(G; x) - D_{e_3}(G; x) &= (D_{e_0}(G; x) - D_{e_3}(G; x)) - (D_{e_0}(G; x) - D_{e_4}(G; x)) \\ &= -(1-x) \sum_{\{e,f\} \in A_4} x^{(\Delta'(e,f)+1)} + \\ &\quad \left(\sum_{\{e,f\} \in A_4} x^{(\Delta'(e,f)+2)} (x^{(2\Delta'(e,f)-1)} - 1) - (x-1) \sum_{\{e,f\} \in A_4} x^{(3\Delta'(e,f))} \right) + \\ &\quad \left(\sum_{\{e,f\} \in A_6} x^{(3\Delta'(e,f)+1)} (x^{\Delta'(e,f)} - 1) - \sum_{\{e,f\} \in A_6} x^{(3\Delta'(e,f))} (x^{(\Delta'(e,f)+1)} - 1) \right) \\ &= -(1-x) \sum_{\{e,f\} \in A_4} x^{(\Delta'(e,f)+1)} + \sum_{\{e,f\} \in A_4} x^{\Delta'(e,f)} (x^{2\Delta'(e,f)} - x^2) + \\ &\quad \sum_{\{e,f\} \in A_6} x^{3\Delta'(e,f)} (1-x). \end{aligned} \quad (12)$$

Result 6. The relations between edge detour indices $D_{e_3}(G)$ and $D_{e_4}(G)$ are:

$$D_{e_4}(G) - D_{e_3}(G) = 2 \sum_{\{e,f\} \in A_4} \Delta'(e,f) + |A_1| - 2|A_4| - |A_6| \quad (13)$$

Proof. We can obtain the result in two ways. The first way is to calculate the first derivative (in $x=1$) of Eqs. 12. The second way is the direct computing by using Eqs. 9 and 10, and replacing them in $D_{e_4}(G) - D_{e_3}(G)$; thus we have:

$$\begin{aligned} D_{e_4}(G) - D_{e_3}(G) &= (D_{e_0}(G) - D_{e_3}(G)) - (D_{e_0}(G) - D_{e_4}(G)) \\ &= 2 \sum_{\{e,f\} \in A_4} \Delta'(e,f) + |A_1| - 2|A_4| - |A_6|. \end{aligned} \quad (14)$$

Now, the relations among edge detour indices and their polynomials are computed for $TUC_4C_8(S)$, $TUC_4C_8(R)$ (for symbols see [9]) and armchair polyhex nanotubes. According to Figure 2, we denote the number of horizontal edges of squares in one row by p and the number of rows by q . Accordingly, $|E(T(p,q))| = 6pq - 2p$. For convenience, we denote $TUC_4C_8(S)$ nanotube by $T(p,q)$ with p being the number of squares in a row and q the number of squares in a column as shown in Figure 2.

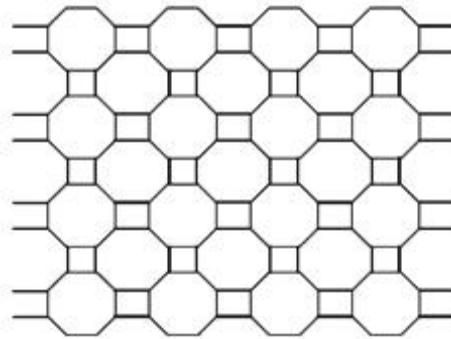


Figure 2. Two dimensional lattice of $TUC_4C_8(S)$ nanotube, $p=4, q=8$.

We denote $TUC_4C_8(R)$ nanotube by $T'(p',q')$ with p' being the number of rhombes in a row and q' the number of rhombs in a column, as shown in Figure 3. Accordingly,

$$|E(T'(p',q'))| = 6p'q' - p'$$

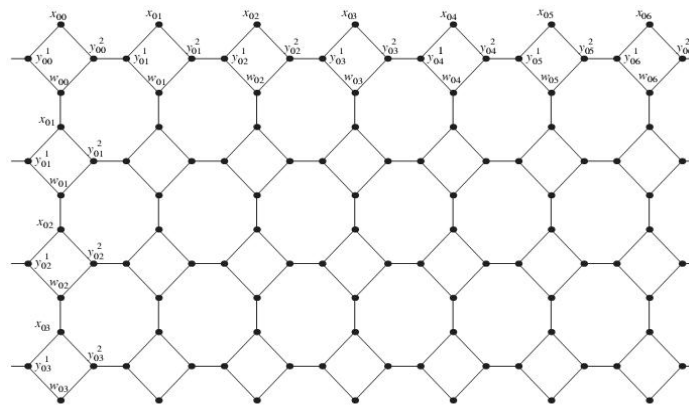


Figure 3. The $T(7,4)$ nanotube.

A single-wall carbon nanotube can be imagined as a graphene sheet rolled at a certain "chiral" angle. An armchair polyhex nanotube, denoted by $TUAC_6[p'',q'']$ [9], is a nanotube with p'' and q'' being the number of hexagons in the length and width, respectively. Also, it has j rows which $1 \leq j \leq q''$ as shown in Figure 4. Accordingly, $|E(T''(p'',q''))| = 6p''q'' + p''$. Next, we denote $TUAC_6[p'',q'']$ nanotube by $T''(p'',q'')$.

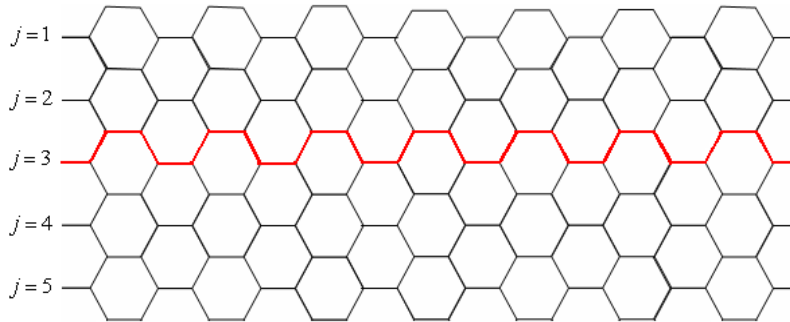


Figure 4. Armchair polyhex nanotube, $TUAC_6[7,5]$, with $1 \leq j \leq 5$ rows.

Theorem 7. The relations among edge detour index polynomials and their indices for $T(p,q)$ nanotubes are:

(I) Relation among edge detour i polynomials

$$D_{e_0}(T(p,q);x) - D_{e_3}(T(p,q);x) = (1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta(e,f)+1)}, \quad (15)$$

$$D_{e_0}(T(p,q);x) - D_{e_4}(T(p,q);x) = (1-x) \sum_{\{e,f\} \subseteq E(G)} x^{(\Delta(e,f)+1)}, \quad (16)$$

$$D_{e_4}(T(p,q);x) - D_{e_3}(T(p,q);x) = -(1-x) \sum_{\{e,f\} \in A_1} x^{(\Delta(e,f)+1)}. \quad (17)$$

(II) Relation among edge detour indices:

$$D_{e_0}(T(p,q)) - D_{e_3}(T(p,q)) = -\left(4p \binom{q}{2} + (q-1) \binom{2p}{2}\right), \quad (18)$$

$$D_{e_0}(T(p,q)) - D_{e_4}(T(p,q)) = -\binom{6pq - 2p}{2}, \quad (19)$$

$$D_{e_4}(T(p,q)) - D_{e_3}(T(p,q)) = 2p(9pq^2 - 7pq - q^2 + 2p). \quad (20)$$

Proof. Due to the Figure 2, the subsets A_3, A_4, A_5 and A_6 are empty and then, we can get results in part I by using the Eqs. 7, 8 and 11.

For results in part II, we can obtain the results in two ways. A way is to calculate the first derivative (in $x=1$) of Eqs. 15, 16 and 17. Let first derive Eqs. 15 to obtain Eqs. 18 (see above):

$$\left((1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta(e,f)+1)} \right)' = - \sum_{\{e,f\} \in A_2} x^{(\Delta(e,f)+1)} + (1-x) \sum_{\{e,f\} \in A_2} (\Delta(e,f)+1) x^{(\Delta(e,f))}$$

By replacing $x=1$ we have

$$\left((1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta(e,f)+1)} \right)'_{x=1} = - \sum_{\{e,f\} \in A_2} 1.$$

Since the subsets A_3, A_4, A_5 and A_6 are empty, $\left| \frac{E(T(p,q))}{2} \right| = |A_1| + |A_2|$. Also, since

$$|E(T(p,q))| = 6pq - 2p, \text{ we have } |A_2| = 4p \binom{q}{2} + (q-1) \binom{2p}{2} \text{ and } |A_1| = 2p(9pq^2 - 7pq - q^2 + 2p).$$

Then

$$\left((1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta(e,f)+1)} \right)'_{x=1} = -\left(4p \binom{q}{2} + (q-1) \binom{2p}{2}\right) \text{ that is Eqs. 18.}$$

Eqs. 19 and 20 can be similarly obtained.

The second way is the direct computing. Due to the Eqs. 8, 9 and 12, we have

$D_{e_0}(T(p, q)) - D_{e_3}(T(p, q)) = -|A_2|$, $D_{e_0}(T(p, q)) - D_{e_4}(T(p, q)) = -(|A_1| + |A_2|)$ and $D_{e_4}(T(p, q)) - D_{e_3}(T(p, q)) = |A_1|$. Then, we can conclude the desired results. ■

Theorem 8. The relations between edge detour polynomials and their indices for $T'(p', q')$ nanotubes are:

(I) Relation among edge detour polynomials

$$D_{e_0}(T'(p', q'); x) - D_{e_3}(T'(p', q'); x) = (1-x) \sum_{\{e, f\} \in A_2} x^{(\Delta(e, f)+1)}, \quad (21)$$

$$D_{e_0}(T'(p', q'); x) - D_{e_4}(T'(p', q'); x) = (1-x) \sum_{\{e, f\} \subseteq E(G)} x^{(\Delta(e, f)+1)}, \quad (22)$$

$$D_{e_4}(T'(p', q'); x) - D_{e_3}(T'(p', q'); x) = -(1-x) \sum_{\{e, f\} \in A_1} x^{(\Delta(e, f)+1)}. \quad (23)$$

(II) Relation among edge detour indices

$$D_{e_0}(T'(p', q')) - D_{e_3}(T'(p', q')) = -\left(p' \left(2 \binom{2q'}{2} + \binom{q'}{2} \right) + (q'-1) \binom{p'}{2} \right), \quad (24)$$

$$D_{e_0}(T'(p', q')) - D_{e_4}(T'(p', q')) = -\binom{6p'q' - p'}{2}, \quad (25)$$

$$D_{e_4}(T'(p', q')) - D_{e_3}(T'(p', q')) = \frac{p'}{2} (36p'q'^2 - 13p'q' - 9q'^2 + 2p') \quad (26)$$

Proof. Due to Figure 2, the subsets A_3 , A_4 , A_5 and A_6 are empty and then, we can get results in part I by using the Eqs. 7, 8 and 11.

For results in part II, we can obtain the results in two ways. The first way is to calculate the first derivative (in $x=1$) of Eqs. 21, 22 and 23. We find Eqs. 24 and then Eqs. 25 and 26 will be obtained by the same procedure.

$$\left((1-x) \sum_{\{e, f\} \in A_2} x^{(\Delta(e, f)+1)} \right)_{x=1} = - \sum_{\{e, f\} \in A_2} x^{(\Delta(e, f)+1)} + (1-x) \sum_{\{e, f\} \in A_2} (\Delta(e, f)+1) x^{(\Delta(e, f))},$$

By replacing $x=1$ we have

$$\left((1-x) \sum_{\{e, f\} \in A_2} x^{(\Delta(e, f)+1)} \right)_{x=1} = - \sum_{\{e, f\} \in A_2} 1.$$

Since the subsets A_3 , A_4 , A_5 and A_6 are empty, $\left(\frac{E(T(p, q))}{2} \right) = |A_1| + |A_2|$. Also, since

$$|E(T'(p', q'))| = 6p'q' - p', \quad \text{we have } |A_2| = p' \left(2 \binom{2q'}{2} + \binom{q'}{2} \right) + (q'-1) \binom{p'}{2} \quad \text{and}$$

$$|A_1| = \frac{p'}{2} (36p'q'^2 - 13p'q' - 9q'^2 + 2p'). \quad \text{Then}$$

$$\left((1-x) \sum_{\{e, f\} \in A_2} x^{(\Delta(e, f)+1)} \right)_{x=1} = - \left(p' \left(2 \binom{2q'}{2} + \binom{q'}{2} \right) + (q'-1) \binom{p'}{2} \right) \quad \text{that it is Eqs. 24.}$$

The second way is the direct computing. Due to the Eqs. 9, 10 and 13, we have

$D_{e_0}(T'(p',q')) - D_{e_3}(T'(p',q')) = -|A_2|$, $D_{e_0}(T'(p',q')) - D_{e_4}(T'(p',q')) = -(|A_1| + |A_2|)$ and $D_{e_4}(T'(p',q')) - D_{e_3}(T'(p',q')) = |A_1|$. Then, we got the desired results. ■

Theorem 2-9. The relations among edge detour polynomials and their indices for $T''(p'',q'')$ nanotubes are:

(I) Relation among edge detour i polynomials

$$D_{e_0}(T''(p'',q'');x) - D_{e_3}(T''(p'',q'');x) = (1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)}, \quad (27)$$

$$D_{e_0}(T''(p'',q'');x) - D_{e_4}(T''(p'',q'');x) = (1-x) \sum_{\{e,f\} \subseteq E(G)} x^{(\Delta'(e,f)+1)}, \quad (28)$$

$$D_{e_4}(T''(p'',q'');x) - D_{e_3}(T''(p'',q'');x) = -(1-x) \sum_{\{e,f\} \in A_1} x^{(\Delta'(e,f)+1)}. \quad (29)$$

(II) Relation among edge detour indices

$$D_{e_0}(T''(p'',q'')) - D_{e_3}(T''(p'',q'')) = -\left(2p'' \binom{2q''}{2} + p'' q''^2\right), \quad (30)$$

$$D_{e_0}(T''(p'',q'')) - D_{e_4}(T''(p'',q'')) = -\binom{6p'' q'' + p''}{2}, \quad (31)$$

$$D_{e_4}(T''(p'',q'')) - D_{e_3}(T''(p'',q'')) = \frac{p''}{2} (36p'' q''^2 - 12p'' q'' - 10q''^2 - 2q'' + p'' - 1) \quad (32)$$

Proof. Due to the Figure 2, the subsets A_3 , A_4 , A_5 and A_6 are empty and then, we can get results in part I by using the Eqs. 7, 8 and 11.

For results in part II, we can obtain the results in two ways. The first way is to calculate the first derivative (in $x=1$) of Eqs. 27, 28 and 29. We find Eqs. 30 and then eqs. 31 and 32 will be obtained by the same procedure.

$$\left((1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)} \right)' = - \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)} + (1-x) \sum_{\{e,f\} \in A_2} (\Delta'(e,f)+1) x^{(\Delta'(e,f))}.$$

By replacing $x=1$ we have

$$\left((1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)} \right)'_{x=1} = - \sum_{\{e,f\} \in A_2} 1.$$

Since the subsets A_3 , A_4 , A_5 and A_6 are empty, $\left(\frac{|E(T(p,q))|}{2} \right)' = |A_1| + |A_2|$. Also, since

$$|E(T''(p'',q''))| = 6p'' q'' + p'', \quad \text{we have} \quad |A_2| = 2p'' \binom{2q''}{2} + p'' \binom{q''+1}{2} + p'' \binom{q''}{2} \quad \text{and}$$

$$|A_1| = \frac{p''}{2} (36p'' q''^2 - 12p'' q'' - 10q''^2 - 2q'' + p'' - 1). \quad \text{Then}$$

$$\left((1-x) \sum_{\{e,f\} \in A_2} x^{(\Delta'(e,f)+1)} \right)'_{x=1} = - \left(2p'' \binom{2q''}{2} + p'' \binom{q''+1}{2} + p'' \binom{q''}{2} \right) = - \left(2p'' \binom{2q''}{2} + p'' q''^2 \right) \quad \text{that it is}$$

Eqs. 30.

The second way is the direct computing. Due to the Eqs. 9, 10 and 13, we have:

$$D_{e_0}(T(p, q)) - D_{e_3}(T(p, q)) = -|A_2|,$$

$$D_{e_0}(T(p, q)) - D_{e_4}(T(p, q)) = -(|A_1| + |A_2|) \text{ and}$$

$$D_{e_4}(T(p, q)) - D_{e_3}(T(p, q)) = |A_1|. \text{ Then we got the desired results. } \blacksquare$$

3. CONCLUSIONS

The relations among edge detour index polynomials of nanotubes $TUC_4C_6(S)$, $TUC_4C_6(R)$ and armchair polyhex nanotubes, and the relations among the edge detour indices of the mentioned nanotubes have been derived, mainly by using the relations between the distances and detours of edges in the molecular graph.

ACKNOWLEDGMENTS.

We thank to Islamic Azad University, Central Tehran Branch, for financial support. Also, the authors are very grateful to Professor Diudea for their comments and suggestions in improving the paper.

REFERENCES

1. H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.*, **69** (1997) 17-20.
2. A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index for trees: theory and applications, *Acta Appl. Math.*, **66** (3) (2001) 211-249.
3. F. Harary, *Graph Theory*, Addison-Wesley, Reading, Massachusetts, 1969.
4. M. V. Diudea, G. Katona, I. Lukovitz and N. Trinajstić, Detour and Cluj-Detour Indices, *Croat. Chem. Acta*, **71** (1998) 459-471.
5. P. E. John, Ueber die Berechnung des Wiener index fuer ausgewaehlte Delta-dimensionale Gitterstrukturen, *MATCH Commun. Math. Comput. Chem.*, **32** (1995) 207-219.
6. R. Jalal Shahkoobi, O. Khormali and A. Mahmiani, The polynomial of detour index for a graph, *World Applied Sciences Journal*, **15** (10) (2011) 1473-1483.
7. A. Mahmiani, O. Khormali and A. Iranmanesh, The edge versions of detour index, *MATCH Commun. Math. Comput. Chem.*, **62** (2) (2009) 419-431.
8. Sh. Safari Sabet, A. Mahmiani, O. Khormali, M. Farmani and Z. Bagheri, On the edge detour index polynomials, *Middle-East Journal of Scientific Research*, **10** (4) (2011) 539-548.
9. M. V. Diudea and Cs. L. Nagy, *Periodic Nanostructures*, Springer, 2007.