The Degree Distance of Armchair Polyhex Nanotubes

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Abstract

The degree distance of a graph which is a degree analogue of the Wiener index of the graph. Let $G = TUVC_6[2p, q]$ be the carbon nanotubes covered by $C_6$, formulas for calculating the degree distance of armchair polyhex nanotubes $TUVC_6[2p, q]$ are provided.

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1 Introduction

Let $G = (V, E)$ be a simple connected graph with the vertex set $V$ and the edge set $E$, $d(x)$ denotes the degree of the vertex $x$. For any $x, y \in V$, $d(x, y)$ denotes the distance (i.e., the number of edges on the shortest path) between $x$ and $y$ and we define $D(x) = \sum_{y \in V(G)} d(x, y)$. The Wiener index of the graph $G$, is equals to the sum of distances between all pairs of vertices of the respective molecular graph, i.e.,

$$W(G) = \sum_{\{x, y\} \in V(G)} d(x, y) \quad (1)$$

The degree distance of a graph which is a degree analogue of the Wiener index of the graph, was introduced by Dobrynin and Kochetova [2] and Gutman [3] as a weighted version of the Wiener index. It was defined as

$$DD(G) = \sum_{x \in V(G)} d(x)D(x) = \sum_{\{x, y\} \in V(G)} d(x, y)(d(x) + d(y)) \quad (2)$$

This parameter has been investigated by several reports. Actually, when $G$ is a tree on $n$ vertices, the parameter is closely related as $DD(G) =$
2W(G) − n(n − 1), for this review see [3]. In [4], A. I. Tomescu characterized the connected unicyclic and bicyclic graphs in terms of the degree sequence, as well as the graphs in these classes minimal with respect to the degree distance are given. In [5], O. Bucicovschi and S. M. Cioabă studied the degree distance of graphs with given order and size, and determined the minimum degree distance of a connected graph of order n and size e. More results in this direction can be found in Refs. [6-10].

Carbon nanotubes were discovered in 1992 by Iijima [11] as multi-walled structures. Two years later, two groups independently discovered the single-walled carbon nanotubes [12,13]. In 1996, Smalley’s group synthesized the aligned single-wall nanotubes [14]. As pointed out by Smalley, a carbon nanotube is a carbon molecule with almost alien property of electrical conductivity and super-steel strength. It is expected that carbon nanotubes can be widely used in many fields. Nanotubes and fullerenes are promising candidates in the development of nanodevices and super-strong composites.

2 Preliminary Notes

Let $G = TUV C_6[2p, q]$ denotes an arbitrary armchair polyhex nanotube in terms of the circumference $p$ and the length $q$. For $k(1 \leq k \leq q)$ is the various levels. An armchair polyhex nanotube with the parameters $p = 10$ is shown in Figure 1.

![Figure 1](image1.png)

Figure 1: The nanotube $TUV C_6[20, q]$
Note that the degrees of vertices in an arbitrary armchair polyhex nanotube are 2 or 3, then the Wiener index \( W(G) \) can be written as

\[
W(G) = \sum_{(u,v) \subseteq V(G)} d_G(u,v) + \sum_{(u,v) \subseteq V(G)} d_G(u,v) + \sum_{(u,v) \subseteq V(G)} d_G(u,v) \tag{3}
\]

The degree distance of \( G = TUVC_6[2p,q] \) can be written as

\[
DD(G) = 2 \sum_{(u,v) \subseteq V(G)} d_G(u,v) + \frac{5}{2} \sum_{(u,v) \subseteq V(G)} d_G(u,v) + 3 \sum_{(u,v) \subseteq V(G)} d_G(u,v) \tag{4}
\]

Further, from the equations (3) and (4), the degree distance of an armchair nanotube can be rewritten as

\[
DD(G) = 3W(G) - \sum_{(u,v) \subseteq V(G)} d_G(u,v) - \frac{1}{2} \sum_{(u,v) \subseteq V(G)} d_G(u,v) \tag{5}
\]

Let \( W_2(G) = \sum_{(u,v) \subseteq V(G)} d_G(u,v), \ W_{2,3}(G) = \sum_{(u,v) \subseteq V(G)} d_G(u,v) \). Therefore, in our calculation we have to calculate \( W_2(G), W_{2,3}(G) \), since \( W(G) \) can be obtained from [17].

Now, we derive a formula for calculating the degree distance of \( TUVC_6[2p,q] \).

3 Main Results

**Lemma 3.1.** Let \( G = TUVC_6[2p,q] \), the Wiener index of \( G \) is

\[
W(G) = \begin{cases} 
\frac{1}{12}p(24p^2q^2 + 2q^4 - 8q^2), & \text{for } q \leq p \text{ and } q \text{ is even;} \\
\frac{1}{12}p(24p^2q^2 + 2q^4 - 8q^2 + 6), & \text{for } q \leq p \text{ and } p \text{ is even, } q \text{ is odd;} \\
\frac{1}{12}p(24p^2q^2 + 2q^4 - 8q^2 - 6), & \text{for } q \leq p, p, q \text{ are odd;} \\
\frac{1}{12}p[p^2(12q^2 - 2p^2 + 8) + 8pq(p^2 + q^2 - 2)], & \text{for } q \geq p \text{ and } p \text{ is even;} \\
\frac{1}{12}p[p^2(12q^2 - 2p^2 + 8) + 8pq(p^2 + q^2 - 2) - 6], & \text{for } q \geq p \text{ and } p \text{ is odd.}
\end{cases}
\]

Let \( s_{0k} \) be the sum of distances from \( v \) to all other vertices at level \( k \), where \( v \) is a vertex of degree 2 at level 1, \( \alpha = \frac{1+(-1)^p}{2}, \beta = \frac{1+(-1)^p}{2} \). Then

\[
s_{0k} = \begin{cases} 
2p^2 + \alpha, & k = 1; \\
2p^2 - \beta + (k-1)^2, & k \leq p \text{ and } k \text{ is even;} \\
2p^2 + \alpha + (k-1)^2, & k \leq p \text{ and } k \text{ is odd} \\
p^2 + 2p(k-1), & k \geq p.
\end{cases}
\]

Let \( \gamma = 1 - (-1)^q \).
Theorem 3.2 Let $G = TUV C_6[2p, q]$.

(1) $p$ is even,

$$DD(G) = \begin{cases} \frac{1}{6}p\{72p^2q^2 + 6q^4 - 48p^2q - 8q^3 - 12q^2 + 8q + 3\gamma\}, & p > q; \\ \frac{1}{4}p^2\{3p^3 - 12p^2q - 18pq^2 - 12q^3 + 4p^2 + 12q^2 + 12pq - 6p \\ + 12q - 4\}, & p \leq q. \end{cases}$$

(2) $p$ is odd,

$$DD(G) = \begin{cases} \frac{1}{6}p\{72p^2q^2 + 6q^4 - 48p^2q - 8q^3 - 12q^2 + 8q - 3\gamma\}, & p > q; \\ \frac{1}{4}p\{3p^4 - 12p^3q - 18p^2q^2 - 12pq^3 + 4p^3 + 12q^2 + 12pq^2 \\ + 12p^2q - 6p^2 + 12pq - 4p + 3\}, & p \leq q. \end{cases}$$

**Proof.** We consider $W_2(G)$ and $W_{2,3}(G)$ and we divide them into two cases.

**Case 1.** The number of $W_2(G)$.

**Subcase 1.1.** $p \leq q$.

**Subcase 1.1.1.** $u$ and $v$ are lying at level 1 and level $q$.

**Subcase 1.1.1.1.** when $p$ is odd.

$$W_{21}(G) = \sum_{1 \leq i < j \leq 2p} d(x_{i1}, x_{1j}) + \sum_{1 \leq i < j \leq 2p} d(x_{qi}, x_{qj}) = 2p(2p^2 - 1)$$

**Subcase 1.1.1.2.** when $p$ is even.

$$W_{21}(G) = \sum_{1 \leq i < j \leq 2p} d(x_{i1}, x_{1j}) + \sum_{1 \leq i < j \leq 2p} d(x_{qi}, x_{qj}) = 2p \times 2p^2$$

**Subcase 1.1.2.** $u$ is lying at level 1, $v$ is lying at level $q$; $u$ is lying at level $q$, $v$ is lying at level 1.

$$W_{22}(G) = \sum_{i=1}^{2p} \sum_{j=1}^{2p} d(x_{i1}, x_{qj}) = 2p(p^2 + 2pq - 2p)$$

Summing up, we arrive at,

$$W_2(G) = W_{21}(G) + W_{22}(G) = \begin{cases} 6p^3 + 4p^2(q - 1) - 2p & p \text{ is odd}; \\ 6p^3 + 4p^2(q - 1), & p \text{ is even}. \end{cases}$$

**Subcase 1.2.** $p \geq q$.

Similar to the discussion in Subcase 1.1, we have,

$$W_2(G) = \begin{cases} 8p^3 + 2p(q - 1)^2 - 4p & p, q \text{ are odd}; \\ 8p^3 + 2p(q - 1)^2 - 2p & p, q \text{ are even}; \\ 8p^3 + 2p(q - 1)^2 - 2p & p \text{ is odd}, q \text{ is even}; \\ 8p^3 + 2p(q - 1)^2, & p \text{ is odd}, q \text{ is even}. \end{cases}$$

**Case 2.** The number of $W_{2,3}(G)$.

**Subcase 2.1.** $p \leq q$.

**Subcase 2.1.1.** when $p$ is even.
Degree distance of armchair polyhex nanotubes

\[ W_{23}(G) = 2 \times 2p \left\{ \sum_{k=2}^{p} (k-1)^2 + (2p^2 - 1) \times \frac{q}{2} + 2p^2 \times \left(\frac{q}{2} - 1\right) \right. \\
+ \left. \sum_{k=p+1}^{q-1} [p^2 + 2p(k-1)] \right\} \\
= \frac{4}{3}p^4 + 4p^3q + 4p^2q^2 - 10p^3 - 12p^2q + \frac{20}{3}p^2 \]

**Subcase 2.1.2.** when \( p \) is odd.

\[ W_{23}(G) = 2 \times 2p \left\{ \sum_{k=2}^{p} (k-1)^2 + (2p^2 - 1 + 2p^2) \times \frac{q-1}{2} + \sum_{k=p+1}^{q-1} [p^2 + 2p(k-1)] \right\} \\
= \frac{4}{3}p^4 + 4p^3q + 4p^2q^2 - 10p^3 - 12p^2q + \frac{20}{3}p^2 + 2p \]

**Subcase 2.2.** \( p \geq q \).

**Subcase 2.2.1.** when \( p \) is even.

**Subcase 2.2.1.1.** when \( q \) is even.

\[ W_{23}(G) = 2 \times 2p \left\{ \sum_{k=2}^{p} (k-1)^2 + (2p^2 - 1) \times (\frac{q}{2} - 1) + 2p^2 \times (\frac{q}{2} - 1) \right\} \\
= 8p^3q + \frac{4}{3}pq^3 - 16p^3 - 6pq^2 + \frac{20}{3}pq \]

**Subcase 2.2.1.2.** when \( q \) is odd.

\[ W_{23}(G) = 2 \times 2p \left\{ \sum_{k=2}^{p} (k-1)^2 + (2p^2 - 1) \times (\frac{q-1}{2}) + 2p^2 \times (\frac{q-1}{2} - 1) \right\} \\
= 8p^3q + \frac{4}{3}pq^3 - 16p^3 - 6pq^2 + \frac{20}{3}pq - 2p \]

**Subcase 2.2.2.** when \( p \) is odd.

**Subcase 2.2.2.1.** when \( q \) is even.

\[ W_{23}(G) = 2 \times 2p \left\{ \sum_{k=2}^{p} (k-1)^2 + 2p^2 \times \frac{q-1}{2} + (2p^2 - 1) \times (\frac{q-1}{2} - 1) \right\} \\
= 8p^3q + \frac{4}{3}pq^3 - 16p^3 - 6pq^2 + \frac{20}{3}pq \]

**Subcase 2.2.2.2.** when \( q \) is odd.

\[ W_{23}(G) = 2 \times 2p \left\{ \sum_{k=2}^{p} (k-1)^2 + 2p^2 \times \frac{4q-1}{2} + (2p^2 - 1) \times (\frac{4q-1}{2} - 1) \right\} \\
= 8p^3q + \frac{4}{3}pq^3 - 16p^3 - 6pq^2 + \frac{20}{3}pq - 2p \]

Combining the above cases, we obtain the results.

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**References**


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