The Wiener and Terminal Wiener indices of trees *

Ya-Hong Chen$^{1,2}$, Xiao-Dong Zhang$^{1\dag}$

$^1$Department of Mathematics, and MOE-LSC,
Shanghai Jiao Tong University
800 Dongchuan road, Shanghai, 200240, P.R. China

$^2$Department of Mathematics, Lishui University
Lishui, Zhejiang 323000, PR China

May 28, 2013

Abstract

Heydari [7] presented very nice formulae for the Wiener and terminal Wiener indices of generalized Bethe trees. It is pity that there are some errors for the formulae. In this paper, we correct these errors and characterize all trees with the minimum terminal Wiener index among all the trees of order $n$ and with maximum degree $\Delta$.

Key words: Wiener index; terminal Wiener index; tree; pendent vertex
AMS Classifications: 05C50, 05C07.

1 Introduction

There are many molecular structure descriptors until now. The Wiener index is one of the most widely known topological descriptors, which has been much studied in both mathematical and chemical literatures (for example, see[2, 4, 3]). Through this paper, we only consider finite, simple and undirected graphs. Let $G = (V(G), E(G))$ be a simple connected graph of order $n$ with vertex set $V(G)$ and edge set $E(G)$. The

*This work is supported by National Natural Science Foundation of China (No:11271256).
\dag Corresponding author (E-mail address: xiaodong@sjtu.edu.cn)
distance between vertices \( v_i \) and \( v_j \) is the minimum number of edges between \( v_i \) and \( v_j \) and denoted by \( d_G(v_i, v_j) \) (or for short \( d(v_i, v_j) \)). The Wiener index of a connected graph \( G \) is defined as the sum of distances between all pairs of vertices:

\[
W(G) = \sum_{v_i, v_j \in V(G)} d(v_i, v_j) = \frac{1}{2} \sum_{v \in V(G)} d_G(v),
\]

where \( d_G(v) \) denotes the distance of a vertex \( v \). For trees, Wiener \[12\] gave a very useful formula for the Wiener index:

\[
W(G) = \sum_{e \in T} n_1(e)n_2(e),
\]

where \( n_1(e) \) and \( n_2(e) \) are the number of vertices of two components of \( T - e \). Recently, Smolenski et al. \[10\] made use of terminal distance matrices to encode molecular structures. Based on these applications, Gutman, Furtula and Petrović \[5\] proposed the concept of terminal Wiener index, which is defined as the sum of distances between all pairs of pendant vertices of trees:

\[
TW(T) = \sum_{1\leq i<j\leq k} d_T(v_i, v_j),
\]

where \( d_T(v_i, v_j) \) is the distance of two pendant vertices \( v_i \) and \( v_j \). Gutman gave a similar formula for the terminal Wiener index of trees

\[
TW(T) = \sum_{e \in T} p_1(e)p_2(e),
\]

where \( n_1(e) \) and \( n_2(e) \) are the number of vertices of two components of \( T - e \). For more information on the Wiener and terminal Wiener indices, the readers may refer to the recent papers \[8, 9, 11\] and the references cited therein.

A generalized Bethe tree (see \[7\]) is a rooted tree whose vertices at the same level have equal degrees. We agree that the root vertex is at level 1 and \( T \) has \( k \) levels, and denote the class of generalized Bethe trees of \( k \) levels by \( B_k \). A Bethe tree \( B_{k,d} \) is a rooted tree of \( k \) levels in which the root vertex has degree \( d \), the vertices at level \( j(2 \leq j \leq k - 1) \) have \( d + 1 \) and the vertices at level \( k \) are the pendant vertices. A regular dendrimer tree \( T_{k,d} \) is a generalized Bethe tree of \( k + 1 \) levels with each nonpendent vertex having degree \( d \). So a regular dendrimer tree belongs to \( B_{k+1} \).

The rest of the paper is organized as follows. In section 2, we present some formulae for the Wiener index of generalized Bethe trees, which correct the errors of
In section 3, a formula for the terminal Wiener indices of trees is obtained. With the formula, the terminal Wiener index of a general Bethe tree is presented, which corrects the errors of \cite{7}. In section 4, the trees with the minimum terminal Wiener index among all the trees of order \( n \) and with maximum degree \( \Delta \) are characterized.

## 2 Wiener index of generalized Bethe trees

Let \( T_1, T_2, \ldots, T_m (m \geq 2) \) be trees with disjoint vertex sets and orders \( n_1, n_2, \ldots, n_m \). Let \( w_i \in V(T_i) \) be the rooted vertex of \( T_i \) for \( i = 1, 2, \ldots, m \). A tree \( T \) on more than two vertices can be regarded as being obtained by joining a new vertex \( w \) to each of the vertices \( w_1, w_2, \ldots, w_m \). Canfield, Robinson and Rouvray \cite{11} elaborated a recursive approach for calculation of the Wiener index of a general tree. Dobrynin, Entringer and Gutman \cite{2} state the result as the following theorem.

**Theorem 2.1** \((\cite{2})\) Let \( T \) be a tree on \( n \geq 3 \) vertices, whose structure is specified above. Then

\[
W(T) = \sum_{i=1}^{m} [W(T_i) + (n - n_i)d_{T_i}(w_i) - n_i^2] + n(n - 1),
\]

where \( d_{T_i}(w_i) \) is the sum of distances between \( w_i \) and all other vertices of \( T_i \) for \( 1 \leq i \leq m \).

Since a generalized Bethe tree is the very special tree whose vertices have the same degree at the same level, Heydari \cite{7} presented a formula for the Wiener index of generalized Bethe trees. The result can be stated as follows:

**Theorem 2.2** \((\cite{7})\) Let \( B_{k+1} \) be a generalized Bethe tree of \( k+1 \) levels. If \( d_1 \) denotes the degree of rooted vertex and \( d_i + 1 \) denotes degree of the vertices on \( i \)th level of \( B_{k+1} \) for \( 1 < i < k \), then the Wiener index of \( B_{k+1} \) is computed as follows:

\[
W(B_{k+1}) = \sum_{i=1}^{k} (n_{i+1} - 1)m_i(n - m_i),
\]

where \( n_{i+1} \) is the number of vertices on the \((i + 1)\)th level of \( B_{k+1} \) and \( m_i \) is the number of all children vertices lying on one side of edge where adjacent a vertex on the \( i \)th level to another vertex on \((i + 1)\)th level of \( B_{k+1} \) for \( 1 \leq i \leq k \).
Unfortunately, this result is not correct. For example[see figure 1]: $B_3$ is a generalized Bethe tree with 9 vertices. It is easy to see that $k = 2, n_2 = 2, n_3 = 6, m_1 = 4, m_2 = 1$. Using the formula as above, we have $W(B_3) = 60$. But actually, the Wiener index of $W(B_3) = 88$. In here, we present a correct formula for the Wiener index of a generalized Bethe tree.

**Theorem 2.3** Let $B_{k+1}$ be a generalized Bethe tree of $k+1$ levels. If $d_1$ denotes the degree of rooted vertex and $d_i + 1$ denotes the degree of vertices on $i$th level of $B_{k+1}$ for $1 < i \leq k$, then

$$W(B_{k+1}) = \sum_{i=1}^{k} n_{i+1}m_i(n - m_i),$$

(3)

where $n_{i+1} = d_1d_2 \cdots d_i$ and $m_i = 1 + \sum_{j=i+1}^{k} \prod_{r=i+1}^{i} d_r$ for $1 \leq i \leq k$.

**Proof.** Let $n_i$ be the number of vertices on the $i$th level of $B_{k+1}$. Thus $n_1 = 1$ and $n_i = d_1d_2d_3 \cdots d_{i-1}$ for $i = 2, 3, \cdots, k + 1$. Denote by $|V(B_{k+1})| = n$. Then

$$n = n_1 + n_2 + \cdots + n_{k+1} = 1 + \sum_{i=1}^{k} \prod_{j=1}^{i} d_j.$$  

Suppose that $u$ on the $i$th level of $B_{k+1}$ for $1 \leq i \leq k$ is the parent of $v$. So all of the children of vertex $v$ are lying one side of edge $e = uv$. Denote by $m_i$ the number of those vertices of the tree. Then

$$m_i = 1 + d_{i+1} + d_{i+1}d_{i+2} + \cdots + d_{i+1}d_{i+2} \cdots d_k = 1 + \sum_{j=i+1}^{k} \prod_{r=i+1}^{i} d_r$$

for $1 \leq i \leq k$. Obviously, $m_k = 1$. Hence the number of vertices where lying two sides of $e$ are equal to $n_1(e) = m_i$ and $n_2(e) = n - m_i$, respectively. Since the number of
edges of $B_{k+1}$ where adjacent a vertex on the $i$th level to another vertex on $(i+1)$th level of $B_{k+1}$ is equal to $n_{i+1}$. By using (1), we have

$$W(B_{k+1}) = \sum_{e \in E(B_{k+1})} n_1(e)n_2(e) = \sum_{i=1}^{k} n_{i+1}m_i(n-m_i)$$

The proof is completed. ■

By using the correct formula (3), it is easy to check that $W(B_3) = 88$. Obviously, the dendrimer tree $T_{k,d}$ is one of the special generalized Bethe trees.

**Corollary 2.4** Let $T_{k,d}$ be a dendrimer tree of $k+1$ levels where degree of the non-pendent vertices is equal to $d$. Then the Wiener index of $T_{k,d}$ is computed as follows:

$$W(T_{k,d}) = \frac{d}{(d-2)^3}[(d-1)^{2k}(kd^2 - 2(k+1)d + 1) + 2d(d-1)^k - 1]. \quad (4)$$

**Proof.** Since the degree of non-pendent vertices of $T_{k,d}$ is equal to $d$, we have $n_1 = 1$, $n_i = d(d-1)^{i-2}$ for $2 \leq i \leq k + 1$, $n = 1 + \frac{d(d-1)^k}{d-2}$ and $m_i = 1 + \frac{(d-1)((d-1)^{k-i}-1)}{d-2}$.

By (3), we have

$$W(T_{k,d}) = \sum_{i=1}^{k} d(d-1)^{i-1}[1 + \frac{(d-1)((d-1)^{k-i}-1)}{d-2}] \frac{d((d-1)^k - 1)}{d-2} - \frac{(d-1)((d-1)^{k-i}-1)}{d-2}$$

$$= \sum_{i=1}^{k} d(d-1)^{i-1} \left[\frac{d-2 + (d-1)((d-1)^{k-i}-1)}{d-2}\right] \frac{[d(d-1)^k - (d-1)^{k-i+1} - 1]}{d-2}$$

$$= \sum_{i=1}^{k} d(d-1)^{i-1} \left[\frac{(d-1)^{k-i+1} - 1}{d-2}\right] \frac{[d(d-1)^k - (d-1)^{k-i+1} - 1]}{d-2}$$

$$= \frac{d}{(d-2)^2} \sum_{i=1}^{k} [(d-1)^k - (d-1)^{i-1}] [d(d-1)^k - (d-1)^{k-i+1} - 1]$$

$$= \frac{d}{(d-2)^2} \sum_{i=1}^{k} [d(d-1)^{2k} - (d-1)^{2k-i+1} - d(d-1)^{k+i-1} + (d-1)^{i-1}]$$

$$= \frac{d}{(d-2)^2} [kd(d-1)^{2k} - \sum_{i=1}^{k}(d-1)^{2k-i+1} - d \sum_{i=1}^{k}(d-1)^{k+i-1} + \sum_{i=1}^{k}(d-1)^{i-1}]$$
\[
\begin{align*}
= \frac{d}{(d-2)^2} & \left[ kd(d-1)^{2k} - \frac{(d-1)^{k+1}((d-1)^k - 1)}{d-2} \right. \\
& \left. - \frac{d(d-1)^k((d-1)^k - 1)}{d-2} + \frac{(d-1)^k - 1}{d-2} \right] \\
= \frac{d}{(d-2)^3} & \left[ (d-1)^{2k} (kd^2 - 2(k+1)d + 1) + 2d(d-1)^k - 1 \right]
\end{align*}
\]

The proof is completed. ■

**Corollary 2.5** The Wiener index of a Bethe tree \( B_{k,d} \) is computed as follows:

\[
W(B_{k,d}) = \frac{d^k}{(d-1)^3} \left[ (k-1)(d-1)(d^k + 1) - 2d(d^{k-1} - 1) \right]
\]

**Proof.** Since degree of the nonpendent vertices of \( B_{k,d} \) is equal to \( d+1 \) except the rooted vertex whose degree is \( d \), we have \( n_1 = 1 \), \( n_{i+1} = d^i \) for \( 1 \leq i \leq k-1 \), \( n = \frac{d^{k-1}-1}{d-1} \) and \( m_i = \frac{d^{k-i}-1}{d-1} \). By (3), we can get

\[
W(B_{k,d}) = \sum_{i=1}^{k-1} d^i \frac{d^k - d^{k-1} - 1}{d-1} \left( \frac{d^{k-i} - 1}{d-1} \right)
\]

\[
= \frac{d^k}{(d-1)^2} \sum_{i=1}^{k-1} (d^k - d^{k-i} - d^i + 1)
\]

\[
= \frac{d^k}{(d-1)^2} \left[ (k-1)(d^k + 1) - \sum_{i=1}^{k-1} d^{k-i} - \sum_{i=1}^{k-1} d^i \right]
\]

\[
= \frac{d^k}{(d-1)^2} \left[ (k-1)(d^k + 1) - 2d(d^{k-1} - 1) \right]
\]

\[
= \frac{d^k}{(d-1)^3} \left[ (k-1)(d-1)(d^k + 1) - 2d(d^{k-1} - 1) \right]
\]

The proof is completed. ■

### 3 Terminal Wiener index of trees

In this section, we consider the terminal Wiener index of trees. For a tree \( T \) with order \( n \geq 3 \) with rooted \( w \), let \( T_1, T_2, \cdots, T_m (m \geq 2) \) be components of \( T - w \) with orders \( n_1, n_2, \cdots, n_m \), respectively, where \( w \) is adjacent to the vertex \( w \) in \( T \) and is the rooted vertex in \( T_i \). Let \( l \) be the number of pendent vertices in \( T \) and \( l_i (1 \leq i \leq m) \) be the number of pendent vertices in \( T_i \). Clearly, \( l_1 + l_2 + \cdots + l_m = l \). We present
a formula for computing the terminal Wiener index of a tree by the terminal Wiener index of subtrees.

**Theorem 3.1** Let $T$ be a tree with order $n \geq 3$, whose structure is described as above. Then

$$TW(T) = \sum_{i=1}^{m} [TW(T_i) + (l - l_i)d'_{T_i}(w_i) - l_i^2] + l^2,$$

where $d'_{T_i}(w_i)$ is the sum of distances between $w_i$ and all other pendent vertices of $T_i$ for $1 \leq i \leq m$.

**Proof.** Let $x_{ij}(1 \leq j \leq l_i)$ be the pendent vertex in $T_i(1 \leq i \leq m)$. Then

$$TW(T) = \sum_{i=1}^{m} TW(T_i) + \sum_{i=2}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{1h}, x_{2k}) + \sum_{i=3}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{1h}, x_{3k}) + \cdots + \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{1h}, x_{m})$$

$$+ \cdots + \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{(m-1)h}, x_{m})$$

$$= \sum_{i=1}^{m} TW(T_i) + \sum_{i=2}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{1h}, x_{ik}) + \sum_{i=3}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{2h}, x_{ik})$$

$$+ \cdots + \sum_{i=m-1}^{m} \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{(m-2)h}, x_{ik}) + \sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{(m-1)h}, x_{m})$$

Since the sum of distances between pendent vertices in each $T_i$ and $T_j$ can be calculated, i.e

$$\sum_{k=1}^{l_i} \sum_{h=1}^{l_i} d(x_{ih}, x_{jk}) = l_j d'_{T_i}(w_i) + l_d'_{T_j}(w_j) + 2l_il_j$$

and $l^2 = (l_1 + l_2 + \cdots + l_m)^2 = \sum_{i=1}^{m} l_i^2 + 2 \sum_{1\leq i<j\leq m} l_il_j$, then we have

$$TW(T) = \sum_{i=1}^{m} TW(T_i) + (l_2 + l_3 + \cdots + l_m)d'_{T_1}(w_1) + (l_1 + l_3 + \cdots + l_m)d'_{T_2}(w_2)$$

$$+ \cdots + (l_1 + l_2 + \cdots + l_{m-1})d'_{T_m}(w_m) + 2 \sum_{1\leq i<j\leq m} l_il_j$$
\[
\sum_{i=1}^{m} TW(T_i) + (l - l_1)d'_{T_1}(w_1) + (l - l_2)d'_{T_2}(w_2) + \cdots \\
+ (l - l_m)d'_{T_m}(w_m) + l^2 - \sum_{i=1}^{m} l_i^2 \\
= \sum_{i=1}^{m} [TW(T_i) + (l - l_i)d'_{T_i}(w_i) - l_i^2] + l^2.
\]

We finish the proof \(\blacksquare\)

With (5), the formulae for the terminal Wiener index of generalized Bethe trees, Bethe trees \(B_{k,d}\) and \(T_{k,d}\) are obtained, which correct the errors of [7].

**Theorem 3.2** Let \(B_{k+1}\) be a generalized Bethe tree of \(k + 1\) levels. Then

\[
TW(B_{k+1}) = \prod_{i=1}^{k} d_i \times (k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{i} d_{k-j+1}).
\]

**Proof.** The pendent vertices of the generalized Bethe tree \(B_{k+1}\) are located on the final level of the tree. Let \(n'\) be the number of pendent vertices of \(B_{k+1}\), then \(n' = d_1d_2 \cdots d_k\). Suppose that \(e = uv\) is an edge of \(B_{k+1}\), and \(u\) is the parent of \(v\) on the \(i\)th level of \(B_{k+1}\) for \(1 \leq i \leq k\). Let \(m'_i\) and \(m''_i\) be the number of pendent vertices of \(B_{k+1}\), lying on the two sides of \(e\), then \(m'_i = d_{i+1}d_{i+2} \cdots d_k\) and \(m''_i = n' - d_{i+1}d_{i+2} \cdots d_k\) for \(1 \leq i \leq k - 1\). Obviously, \(m'_k = 1\) and \(m''_k = n' - 1\).

Since we have mentioned in Theorem 2.2 that \(n_{i+1}\) which stands for the number of edges where adjacent a vertex on the \(i\)th level to another vertex on the \((i + 1)\)th level of \(B_{k+1}\) is equal to \(d_1d_2 \cdots d_i\) for \(1 \leq i \leq k + 1\), by using (2), we have

\[
TW(B_{k+1}) = \sum_{e \in E(B_{k+1})} p_1(e)p_2(e) \\
= \sum_{i=1}^{k-1} n_{i+1}m'_im''_i + n'm'_km''_k \\
= \sum_{i=1}^{k-1} n_{i+1}d_{i+1}d_{i+2} \cdots d_k(n' - d_{i+1}d_{i+2} \cdots d_k) + n'(n' - 1) \\
= \sum_{i=1}^{k-1} d_1d_2 \cdots d_id_{i+1}d_{i+2} \cdots d_k(d_1d_2 \cdots d_k - d_{i+1}d_{i+2} \cdots d_k) + d_1d_2 \cdots d_k(d_1d_2 \cdots d_k - 1)
\]
\[(k - 1)(\prod_{i=1}^{k} d_i)^2 - \prod_{i=1}^{k} d_i \sum_{i=1}^{k-1} d_{i+1}d_{i+2} \cdots d_k + \prod_{i=1}^{k} d_i (\prod_{i=1}^{k} d_i - 1)\]
\[= \prod_{i=1}^{k} d_i \times [(k - 1)(\prod_{i=1}^{k} d_i) + \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} d_{i+1}d_{i+2} \cdots d_k]\]
\[= \prod_{i=1}^{k} d_i \times (k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{d_{k-j+1}})\]

The proof is completed. ■

From Theorem 3.2, we can get the terminal Wiener index of \(T_{k,d}\).

**Corollary 3.3** Let \(T_{k,d}\) be a dendrimer tree of \(k + 1\) levels where degree of the nonpendent vertices is equal to \(d\). Then the terminal Wiener index of \(T_{k,d}\) is computed as follows:

\[TW(T_{k,d}) = d(d - 1)^{k-1}[kd(d - 1)^{k-1} + \frac{1 - (d - 1)^k}{d - 2}]\]

**Proof.** Since degree of the nonpendent vertices of \(T_{k,d}\) is equal to \(d\), it is easy to see that \(d_1\) is equal to \(d\) and \(n_i\) is equal to \(d - 1\) for \(2 \leq i \leq k\). Then

\[n' = \prod_{i=1}^{k} d_i = d(d - 1)^{k-1}\]

and

\[\sum_{i=1}^{k-1} \prod_{j=1}^{d_{k-j+1}} = \sum_{i=1}^{k-1} d_{i+1}d_{i+2} \cdots d_k\]
\[= \sum_{i=1}^{k-1} (d - 1)^{k-i}\]
\[= \frac{(d - 1)[(d - 1)^{k-1} - 1]}{d - 2}.

By using (6), we have

\[TW(T_{k,d}) = d(d - 1)^{k-1}[kd(d - 1)^{k-1} - 1 - \frac{(d - 1)[(d - 1)^{k-1} - 1]}{d - 2}]\]
\[= d(d - 1)^{k-1}[kd(d - 1)^{k-1} + \frac{1 - (d - 1)^k}{d - 2}].

The proof is completed. ■
Corollary 3.4 Let $B_{k,d}$ be a Bethe tree of $k$ levels. Then

$$TW(B_{k,d}) = \frac{d^{k-1}}{d-1}[d^{k-1}(kd-k-d)+1].$$

Proof. Since $B_{k,d}$ is a Bethe tree of level $k$, we replace $k$ in formula (6) by $k - 1$. According to the definition of the Bethe tree $B_{k,d}$, it is easy to see that $\prod_{i=1}^{k-1} d_i = d^{k-1}$ and

$$\sum_{i=1}^{k-2} \prod_{j=1}^{i} d_{k-j} = \sum_{i=1}^{k-2} d_{i+1}d_{i+2}\cdots d_{k-1}$$

$$= \sum_{i=1}^{k-2} d^{k-i-1}$$

$$= \frac{d[d^{k-2} - 1]}{d - 1}.$$

By using (6), we have

$$TW(B_{k,d}) = d^{k-1}[(k - 1)d^{k-1} - 1 - \frac{d(d^{k-2} - 1)}{d - 1}]$$

$$= d^{k-1}[(k - 1)d^{k-1} - \frac{d^{k-1} - 1}{d - 1}]$$

$$= \frac{d^{k-1}}{d - 1}[(k - 1)(d - 1)d^{k-1} - d^{k-1} + 1]$$

$$= \frac{d^{k-1}}{d - 1}d^{k-1}(kd-k-d) + 1].$$

The proof is completed. ■

4 Terminal Wiener index versus maximum degree in trees

Let $T(n, \Delta)$ denote the set of all the trees of order $n$ and with maximum degree $\Delta$. In this section, we will characterize the trees with the minimum terminal Wiener index in $T(n, \Delta)$.
In order to prove our main result, we introduce a tree transformation. Let $T_{a,b}$ and $T_{a-1,b+1}$ be the trees depicted in Figure 2, where $b > a \geq 1$ are integers and $R$ is a rooted tree with root $r$ and at least two vertices. Gutman, Vukičević and Petrović proved

**Lemma 4.1** Let $b > a \geq 1$. Then

$$W(T_{a,b}) < W(T_{a-1,b+1}).$$

However, the above result is not true for terminal Wiener index. In fact,

**Lemma 4.2** If $b > a > 1$, then

$$TW(T_{a,b}) = TW(T_{a-1,b+1}).$$

**Proof.** Suppose that there are $k$ pendent vertices of $R$ which are labelled by $x_1, x_2, \ldots, x_k$. Then

$$TW(T_{a,b}) = \sum_{1 \leq i < j \leq k} d(x_i, x_j) + \sum_{i=1}^{k} d(x_a, x_i) + \sum_{i=1}^{k} d(v_b, x_i) + a + b$$

$$= \sum_{1 \leq i < j \leq k} d(x_i, x_j) + 2 \sum_{i=1}^{k} d(r, x_i) + (a + b)k + a + b$$

and

$$TW(T_{a-1,b+1}) = \sum_{1 \leq i < j \leq k} d(x_i, x_j) + \sum_{i=1}^{k} d(u_{a-1}, x_i) + \sum_{i=1}^{k} d(x_a, x_i) + a + b$$

$$= \sum_{1 \leq i < j \leq k} d(x_i, x_j) + 2 \sum_{i=1}^{k} d(r, x_i) + (a + b)k + a + b.$$ 

It is easy to see that $TW(T_{a,b}) = TW(T_{a-1,b+1})$. The proof is completed. 

**Lemma 4.3** If $b > a = 1$, then

$$TW(T_{a,b}) > TW(T_{a-1,b+1}).$$

11
Proof. Suppose that there are \( k \) pendant vertices of \( R \) which are labelled by \( x_1, x_2, \ldots, x_k \). Then

\[
TW(T_{a,b}) = \sum_{1 \leq i < j \leq k} d(x_i, x_j) + 2 \sum_{i=1}^{k} d(r, x_i) + (b + 1)k + b + 1
\]

and

\[
TW(T_{a-1,b+1}) = \sum_{1 \leq i < j \leq k} d(x_i, x_j) + \sum_{i=1}^{k} d(r, x_i) + (b + 1)k.
\]

So \( TW(T_{a,b}) - TW(T_{a-1,b+1}) = \sum_{i=1}^{k} d(r, x_i) + b + 1 > 0 \). The proof is completed. \( \blacksquare \)

A tree is said to be starlike of degree \( k \) if exactly one of its vertices has degree greater than two, and the degree is equal to \( k \geq 3 \).

**Theorem 4.4** If \( T \) is a tree in \( \mathcal{T}(n, \Delta)(\Delta \geq 3) \), then

\[
TW(T) \geq (n - 1)(\Delta - 1)
\]

with equality if and only if \( T \) is starlike of order \( n \) with the maximum degree \( \Delta \).

Proof. Since \( T \in \mathcal{T}(n, \Delta) \), there exists at least one vertex labelled by \( v \) such that \( d(v) = \Delta \). So there are \( \Delta \) branches of \( T - v \). If \( T \) is not a starlike tree, there exist some branches of \( T \) at \( v \) that are not paths. Hence by Lemmas 4.2 and 4.3 there exist a starlike tree \( T_1 \) of order \( n \) with the maximum degree \( \Delta \) such that \( TW(T) > TW(T_1) \). Moreover, any two starlike trees of order \( n \) with the maximum degree \( \Delta \) have the same terminal Wiener index, which is equal to \( (n - 1)(\Delta - 1) \). Hence the proof is completed. \( \blacksquare \)

**References**

[1] E. R. Canfield, R. W. Robinson and D. H. Rouvray, Determination of the Wiener molecular branching index for the general tree, *J.Comput.Chem.* 6 (1985) 598-609.

[2] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* 66 (2001) 211-249.
[3] I. Gutman, S. Klavzar, B. Mohar (eds.), Fifty years of the Wiener index, *MATCH Commun. Math. Comput. Chem.* 35 (1997) 1-159.

[4] I. Gutman, S. Klavzar, B. Mohar (eds.), Fiftieth anniversary of the Wiener index. *Discrete Appl. Math.* 80 (1997) 1-113.

[5] I. Gutman, B. Furtula, M. Petrović, Terminal Wiener index, *J. Math. Chem.* 46 (2009) 522-531.

[6] I. Gutman, D. Vukičević, J. Žerovnik, A class of modified Wiener indices, *Croat. Chem. Acta* 77 (2004) 103-109.

[7] A. Heydari, On the Wiener and Terminal Wiener index of Generalized Bethe Trees, *MATCH Commun. Math. Comput. Chem.* 69 (2013) 141-150.

[8] A. Heydari, I. Gutman, On the terminal Wiener index of thorn graphs, *Kragujevac J. Sci.* 32 (2010) 57-64.

[9] N.S. Schmuck, S.G. Wagner, H. Wang, Greedy trees, caterpillars, and Wiener-type graph invariants, *MATCH Commun. Math. Comput. Chem.* 68 (2012) 273-292.

[10] E. A. Smolenskii, E. V. Shuvalova, L. K. Maslova, I. V. Chuvaeva, M. S. Molchanova, Reduced matrix of topological distances with a minimum number of independent parameters: distance vectors and molecular codes, *J. Math. Chem.* 45 (2009) 1004-1020.

[11] L.A. Székely, H. Wang, T. Wu, The sum of the distances between the leaves of a tree and the 'semi-regular' property, *Discrete Math.* 311 (2011) 1197-1203.

[12] H. Wiener, Structural determination of paraffin boiling points, *J. Amer. Chem. Soc.* 69 (1947) 17-20.