MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 609-622

ISSN 0340 - 6253

Trees with extremal Wiener indices *

Sujuan Wang [a], Xiaofeng Guo [b, a, †]

[a] School of Mathematical Sciences, Xiamen University, Xiamen Fujian 361005, P. R. China

[b] College of Mathematics and System Sciences, Xinjiang University, Wulumuqi Xinjiang 830046, P. R. China

(Received December 10, 2007)

Abstract

The Wiener index of a connected graph is the sum of distances for all pairs of vertices. In this paper, we consider the trees with order n, diameter d or maximum degree Δ, and extremal Wiener indices. We obtain the tree with minimum Wiener index among all the trees of order n and with diameter d, and the trees with minimum and maximum Wiener indices among all the caterpillar trees of order n and with diameter d. We also obtain the tree with maximum Wiener index among all the trees of order n and with maximum degree Δ, and the trees with the second and the third maximum Wiener indices among all the trees of order n, whose vertices are of degree 1 or Δ.

* The project supported by NFSC.

† Corresponding author. *E-mail:* xfguo@xmu.edu.cn

1 Introduction

The molecular-graph-based quantity W, introduced by Harold Wiener [1] in 1947, is nowadays known as the name *Wiener index* or *Wiener number*. For a connected graph G, let $V(G)$ denote the set of vertices and $E(G)$ the set of edges. Then the Wiener index of G, denoted by $W(G)$, is defined by

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v|G) \tag{1}$$

where $d(u,v|G)$ is the distance between vertices of u and v in G, and the summation goes over all pairs of vertices in $V(G)$.

Let T be a tree and $e = uv$ an edge of T. Denote by $n_u(e|T)$ (resp. $n_v(e|T)$) the number of vertices of T lying on one side of the edge e, closer to vertex u (resp. v). Then the Wiener index of T also satisfies the following relation [1]:

$$W(T) = \sum_{e=uv} n_u(e|T) \cdot n_v(e|T) \tag{2}$$

in which the summation goes over all edges of T.

There is a lot of mathematical and chemical literature on the Wiener index, especially on the Wiener index of trees. A survey of known results and open problems was given by Dobrynin et al. [2]. It is of great interest to identify the graphs with extremal Wiener indices for both chemical applications and mathematics, and many results have been obtained [3—11]. One of the most well known results is that [3,4] among all the trees of order n, the Wiener index is maximized by the path P_n and minimized by the star S_n.

A maximal subtree of a tree T containing a vertex v as an end vertex will be called a *branch* of T at v. A vertex of a tree T, having degree 3 or greater, is called a *branching point* of T. A tree T is said to be a *starlike tree* if exactly one of its vertices has degree greater than two, viz. T has exactly one branching point.

A *rooted tree* T has one of its vertices, called the *root*, distinguished from the others.

The *dumbbell* $D(n,a,b)$ consists of the path P_{n-a-b} together with a independent vertices adjacent to one pendent vertex of P_{n-a-b} and b independent vertices to the other pendent vertex.

A *caterpillar tree* is a tree, the deletion of whose pendent vertices produces a path. Let $C_\Delta(n)$ denote the caterpillar tree of order n, whose vertices are of degree 1 or Δ.

A *dendrimer* of degree Δ on n vertices, $D_{n,\Delta}$, is a tree with maximum degree Δ defined inductively as follows. The tree $D_{1,\Delta}$ consists of a single vertex labelled 1. The tree $D_{n,\Delta}$ has vertex set $\{1, 2, \ldots, n\}$ and is obtained by attaching a leaf n to the smallest numbered vertex of $D_{n-1,\Delta}$, which has degree $< \Delta$.

The diameter of a graph is an important graph-theoretical parameter. Let $\mathcal{G}(n, d)$ denote the set of all the connected graphs of order n and with diameter d. Plesnik [11] obtained the graphs (may not be unique) with minimum Wiener index in $\mathcal{G}(n, d)$ ($d \leq n-1$). When $d < n-1$, they are cycle-containing graphs. Wagner [14] obtained the trees with maximum Wiener index among all the trees with n edges and diameter ≤ 4.

Let $\mathcal{T}(n, \Delta)$ denote the set of all the trees of order n and with maximum degree Δ, and $\mathcal{T}_{1,\Delta}(n)$ the set of all the trees of order n, whose vertices are of degree 1 or Δ. Liu et al. [5] showed that the dendrimer $D_{n,\Delta}$ is the unique tree with minimum Wiener index in $\mathcal{T}(n, \Delta)$. Later, by using different approaches, Fishermann et al. [6] and Jelen et al. [7] independently characterized the tree with minimum Wiener index among all the trees of order n and with maximum degree $\leq \Delta$. In fact, it is also the dendrimer $D_{n,\Delta}$. Fishermann et al. [6] also showed that the tree $C_\Delta(n)$ is the unique tree with maximum Wiener index in $\mathcal{T}_{1,\Delta}(n)$.

Let $\mathcal{T}^*(n, d)$ (resp. $\mathcal{C}^*(n, d)$) denote the set of all the trees (resp. caterpillar trees) of order n and with diameter d. Clearly, $\mathcal{C}^*(n, d) \subseteq \mathcal{T}^*(n, d)$.

In this paper, by using some tree transformations which strictly increase or decrease the Wiener index of trees, we obtain the tree with minimum Wiener index in $\mathcal{T}^*(n, d)$ ($2 \leq d \leq n-1$), the trees with minimum and maximum Wiener indices in $\mathcal{C}^*(n, d)$, and additionally the tree with minimum Wiener index among all the trees of order n and with diameter $\geq d$. And we also obtain the tree with maximum Wiener index in $\mathcal{T}(n, \Delta)$, and the trees with the second and the third maximum Wiener indices in $\mathcal{T}_{1,\Delta}(n)$.

The structures of the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$ might be quite different according to different values of n and d, and so we can't characterize them in a general way. However, for some special values of d, $2 \leq d \leq 4$ or $n-3 \leq d \leq n-1$, the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$ are also determined in this paper.

2 Wiener index versus diameter in trees

In this section, we will characterize the trees with extremal Wiener indices in $\mathcal{T}^*(n,d)$ and in $\mathcal{C}^*(n,d)$. In addition, we also obtain the trees with extremal Wiener indices among all the trees of order n and with diameter at least d.

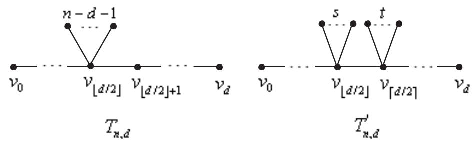


Figure 1: The trees $T_{n,d}$ and $T^{'}_{n,d}$.

Let n and d be two integers satisfying $n > d \geq 2$. Let $T_{n,d}$ be the tree consisting of a path $P = v_0v_1 \ldots v_d$ together with $n-d-1$ independent vertices all adjacent to $v_{\lfloor d/2 \rfloor}$. When d is odd, let $T^{'}_{n,d}$ be the tree consisting of a path $P = v_0v_1 \ldots v_d$ together with s independent vertices adjacent to $v_{\lfloor d/2 \rfloor}$ and t independent vertices adjacent to $v_{\lceil d/2 \rceil}$, where $s \geq 0$, $t \geq 0$ and $s+t = n-d-1$ (see figure 1). When d is odd, $\lfloor d/2 \rfloor + 1 = \lceil d/2 \rceil$. So if $s = 0$ or $t = 0$, then $T_{n,d} \cong T^{'}_{n,d}$ (d is odd).

The following theorem presents the tree with minimum Wiener index in $\mathcal{T}^*(n,d)$.

Theorem 2.1 If T is a tree in $\mathcal{T}^*(n,d)$ $(2 \leq d \leq n-1)$, then

$$W(T) \geq W(T_{n,d}).$$

The equality holds if and only if $T \cong T_{n,d}$.

In order to prove this conclusion, some preparations are needed.

Lemma 2.2 [12] Let T be a tree of order n and $e = v_0v_1 \in E(T)$. Let T_i, i=0,1, be the components of $T - e$ containing v_i with $|V(T_i)| = n_i$, and let $u_1, u_2, \ldots, u_t$ be pendent vertices of T, which is adjacent to v_1. Then, $W(T + \sum_{j=1}^{t}(-v_1u_j + v_0u_j)) - W(T) = t(n_1 - n_0 - t)$.

By lemma 2.2, the following is immediate.

Lemma 2.3 Let $d \geq 3$ be an odd number. And let $T_{n,d}$ and $T^{'}_{n,d}$ be the trees described as above. Then, $W(T^{'}_{n,d}) \geq W(T_{n,d})$, with the equality if and only if $T^{'}_{n,d} \cong T_{n,d}$.

Here, we need to use two tree transformations. The first one is the inner-moving transformation.

Definition 2.4 Let T_{11} be the tree consist of a path $u_0u_1u_2 \cdots u_t$ of length t and rooted trees X_i with roots u_i, $l \le i \le t-1$, $1 \le l < \lfloor t/2 \rfloor$, $|V(X_l)| > 1$, and $|V(X_i)| \ge 1$ for $l+1 \le i \le t-1$. Let T_{12} be the tree obtained from T_{11} by moving the rooted tree X_l to u_{l+1} such that the root of X_l is identified with u_{l+1} (see figure 2). Then T_{12} is said to be obtained from T_{11} by a step of *inner-moving transformation* or *i.m.t.* for short.

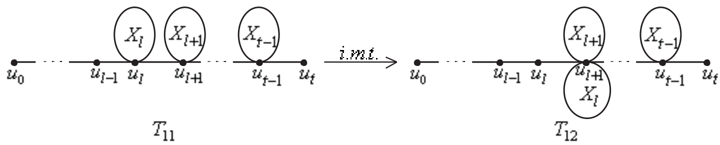


Figure 2: The inner-moving transformation of the tree T_{11}.

Lemma 2.5 The inner-moving transformation decreases the Wiener index, viz.

$$W(T_{11}) > W(T_{12}).$$

Proof. Set $a_i = |V(X_i) \setminus u_i|$ $(l \le i \le t-1)$. Then, $a_l > 0$ and $a_i \ge 0$ for $l+1 \le i \le t-1$. Using formula (2), we consider the difference $W(T_{11}) - W(T_{12})$. Comparing the structures of T_{11} and T_{12}, we can get that $n_u(e|T_{11}) \cdot n_v(e|T_{11}) = n_u(e|T_{12}) \cdot n_v(e|T_{12})$ holds for every edge $e = uv$ in $E(T_{11})$ and $E(T_{12})$, except that of $e = u_l u_{l+1}$. Therefore,

$$W(T_{11}) - W(T_{12})$$

$$\begin{aligned} &= n_{u_l}(e|T_{11}) \cdot n_{u_{l+1}}(e|T_{11}) - n_{u_l}(e|T_{12}) \cdot n_{u_{l+1}}(e|T_{12}) \qquad (\text{where } e = u_l u_{l+1}) \\ &= n_{u_l}(e|T_{11}) \cdot n_{u_{l+1}}(e|T_{11}) - (n_{u_l}(e|T_{11}) - a_l) \cdot (n_{u_{l+1}}(e|T_{11}) + a_l) \\ &= a_l \cdot (n_{u_{l+1}}(e|T_{11}) - n_{u_l}(e|T_{11}) + a_l) \end{aligned}$$

Clearly, $n_{u_l}(e|T_{11}) - a_l = l + 1$. Noticing that $a_i \ge 0$ $(l+1 \le i \le t-1)$, we have $n_{u_{l+1}}(e|T_{11}) \ge t - l$. So, $n_{u_{l+1}}(e|T_{11}) - n_{u_l}(e|T_{11}) + a_l \ge (t-l) - (l+1) = t - 2l - 1$.

As $1 \le l < \lfloor t/2 \rfloor \le t/2$, we have $l \le t/2 - 1$. Then, $t - 2l - 1 \ge 1 > 0$. And so $n_{u_{l+1}}(e|T_{11}) - n_{u_l}(e|T_{11}) + a_l > 0$. Note that $a_l > 0$. Therefore, $W(T_{11}) > W(T_{12})$. ■

The second tree transformation we need is the edge-growing transformation, which had been used by Dong and Guo [12] for ordering trees by their Wiener indices.

Definition 2.6 Let T_{21} be a tree of order n and $T_{21} \ne S_n$. Let $e = uv$ be a non-pendent edge of T_{21}, and T_1 and T_2 be the two components of $T_{21} - e$, $u \in T_1$, $v \in T_2$. T_{22} is the tree obtained from T_{21} in the following way:

(1) Contract the edge $e = uv$;
(2) Add a pendent edge to the vertex $u(= v)$;
The procedures (1) and (2) are called the *edge-growing transformation* of T_{21} (on edge e) or *e.g.t.* of T_{21} (on edge e) for short (see figure 3).

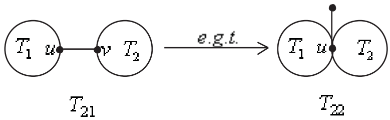


Figure 3: The edge-growing transformation of the tree T_{21}.

Lemma 2.7 [12] The edge-growing transformation decreases the Wiener index, viz.

$$W(T_{21}) > W(T_{22}).$$

Now we come to the proof of Theorem 2.1.

Proof of Theorem 2.1. Let T be a tree in $\mathcal{T}^*(n, d)$, and let $P = v_0v_1 \cdots v_d$ be a longest path in T. Clearly, $d_T(v_0) = d_T(v_d) = 1$. Let X_i be the component of $T - E(P)$ containing v_i, $i = 1, 2, \cdots, d-1$, which is a rooted tree with root v_i.

By *e.g.t.* for all the non-pendent edges of T not on P, T can be transformed to a caterpillar tree T^* such that every rooted tree X_i becomes a star (see figure 4). By lemma 2.7, $W(T) \geq W(T^*)$, with the equality if and only if $T \cong T^*$.

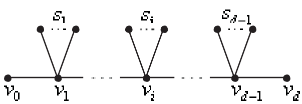


Figure 4: A caterpillar tree in the proof of theorem 2.1.

In addition, by *i.m.t.*, T^* can be transformed into either $T_{n,d}$ or $T'_{n,d}$ (if d is odd). Now it follows from lemmas 2.3 and 2.5 that $W(T) \geq W(T^*) \geq W(T_{n,d})$, with the equality if and only if $T \cong T^* \cong T_{n,d}$. ■

Corollary 2.8 If T is a tree of order n and with diameter at least d $(2 \leq d < n)$, then

$$W(T_{n,d}) \leq W(T) \leq W(P_n). \qquad (*)$$

The lower bound is realized if and only if $T \cong T_{n,d}$ and the upper bound if and only if $T \cong P_n$.

Proof. Note that the diameter of the path P_n is $n-1 \geq d$. As P_n maximizes the Wiener index among all the trees of order n, the right-hand side inequality in $(*)$ holds obviously.

Now we prove the left-hand side inequality in $(*)$. If T is a tree with diameter greater than d, then T can be transformed into a tree (say $T^{'}$) with diameter d by a number of *e.g.t.*. By lemma 2.7, $W(T) > W(T^{'})$. So, we can conclude that if T minimizes the Wiener index among all the trees of order n and with diameter $\geq d$, then T must be a tree of order n and with diameter d. Then, the left-hand side inequality in $(*)$ follows from theorem 2.1. ■

Now, we consider the trees in $\mathcal{C}^*(n,d)$. Clearly, $\mathcal{C}^*(n,d) \subseteq \mathcal{T}^*(n,d)$, and $T_{n,d} \in \mathcal{C}^*(n,d)$. The tree with minimum Wiener index in $\mathcal{C}^*(n,d)$ is also the tree $T_{n,d}$. In addition, the tree with maximum Wiener index in $\mathcal{C}^*(n,d)$ can also be characterized.

Let $\mathcal{L}(n,l)$ $(2 \leq l \leq n-1)$ denote the set of all the trees of order n and with l pendent vertices. The following lemma gives the tree with maximum Wiener index in $\mathcal{L}(n,l)$, which was obtained by Shi [8] and later independently by Entringer [9].

Lemma 2.9 [8,9] If T is a tree in $\mathcal{L}(n,l)$ $(2 \leq l \leq n-1)$, then

$$W(T) \leq W(D(n, \lfloor l/2 \rfloor, \lceil l/2 \rceil)).$$

The equality holds if and only if $T \cong D(n, \lfloor l/2 \rfloor, \lceil l/2 \rceil)$.

The above lemma can be used to obtain the tree with maximum Wiener index in $\mathcal{C}^*(n,d)$.

Theorem 2.10 If T is a tree in $\mathcal{C}^*(n,d)$ $(2 \leq d \leq n-1)$, then

$$W(T_{n,d}) \leq W(T) \leq W(D(n, \lfloor (n-d+1)/2 \rfloor, \lceil (n-d+1)/2 \rceil)). \qquad (\star)$$

The lower bound is realized if and only if $T \cong T_{n,d}$ and the upper bound if and only if $T \cong D(n, \lfloor (n-d+1)/2 \rfloor, \lceil (n-d+1)/2 \rceil)$.

Proof. The left-hand side inequality in $(\star)$ follows immediately from theorem 2.1.

Now we prove the right-hand side inequality in $(\star)$. By lemma 2.9, $D(n, \lfloor (n-d+1)/2 \rfloor, \lceil (n-d+1)/2 \rceil)$ is the unique tree with maximum Wiener index in $\mathcal{L}(n, n-d+1)$. It is not difficult to see that $D(n, \lfloor (n-d+1)/2 \rfloor, \lceil (n-d+1)/2 \rceil) \in \mathcal{C}^*(n,d) \subseteq \mathcal{L}(n, n-d+1)$. So, $D(n, \lfloor (n-d+1)/2 \rfloor, \lceil (n-d+1)/2 \rceil)$ is also the unique tree with maximum Wiener index in $\mathcal{C}^*(n,d)$. Thus, the right-hand side inequality in $(\star)$ also holds. ■

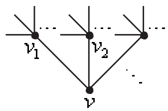
Now we consider the trees with maximum Wiener index in $\mathcal{T}^*(n,d)$ $(2 \leq d \leq n-1)$.

Here, the trees with maximum Wiener index in $\mathcal{T}^*(n,d)$ are determined for $2 \le d \le 4$ or $n-3 \le d \le n-1$.

When the diameter $d = \bar{d} \in \{2, 3, n-1, n-2\}$, the trees in $\mathcal{T}^*(n,\bar{d})$ are all caterpillar trees, viz. $\mathcal{T}^*(n,\bar{d}) = \mathcal{C}^*(n,\bar{d})$. Then, by theorem 2.10, the unique tree with maximum Wiener index in $\mathcal{T}^*(n,\bar{d})$ is the tree $D(n, \lfloor (n-\bar{d}+1)/2 \rfloor, \lceil (n-\bar{d}+1)/2 \rceil)$.

When $d = 4$, the trees with maximum Wiener index in $\mathcal{T}^*(n,4)$ can be obtained from the result of Theorem 3 in Wagner [14]. But there is a little mistake in it (see the remark after Theorem 2.12). Here, we will restate the result as Theorem 2.12.

Definition 2.11 [14] Let $(c_1, c_2, \dots, c_t)$ be a partition of $n-1$ $(n > 1)$. A tree with diameter ≤ 4 assigned to this partition is the tree



where $v_1, v_2, \dots, v_t$ have degrees $c_1, c_2, \dots, c_t$ respectively. It has exactly $n-1$ edges (viz. n vertices). The tree itself is denoted by $S(c_1, c_2, \dots, c_t)$.

Set $k = \lfloor \sqrt{n-1} \rfloor$ $(n > 1)$. If $k^2 + k \ge n-1$, set $T_m = S(\underbrace{k, \dots k}_{k^2+k-n+1}, \underbrace{k+1, \dots, k+1}_{n-k^2-1})$. If $k^2+k \le n-1$, set $T'_m = S(\underbrace{k, \dots, k}_{k^2+2k-n+2}, \underbrace{k+1, \dots, k+1}_{n-k^2-k-1})$. Notice that when $k^2+k = n-1$, T_m and T'_m are non-isomorphic trees with $W(T_m) = W(T'_m) = 2k^3(k+1)$.

Theorem 2.12 [14] Let T be a tree with n vertices and diameter ≤ 4. Set $k = \lfloor \sqrt{n-1} \rfloor$.
(1) If $k^2 + k > n-1$, then $W(T) \le W(T_m)$, with the equality if and only if $T \cong T_m$.
(2) If $k^2 + k < n-1$, then $W(T) \le W(T'_m)$, with the equality if and only if $T \cong T'_m$.
(3) If $k^2 + k = n-1$, then $W(T) \le W(T_m) = W(T'_m)$, with the equality if and only if $T \cong T_m$ or $T \cong T'_m$.

Remark: From the result of Theorem 3 in [14], we get that when $k^2 + k = n-1$, the tree with maximum Wiener index among all the trees with n vertices and diameter ≤ 4 is the tree T'_m. But, in fact, when $k^2 + k = n-1$, T_m and T'_m are both the trees with maximum Wiener index. In other words, Theorem 3 of [14] misses out the tree T_m for the case when $k^2 + k = n-1$.

It is not difficult to see that, if $n \ge 5$, $k = \lfloor \sqrt{n-1} \rfloor \ge 2$, and T_m and T'_m are trees with diameter 4. From theorem 2.12, we can conclude that the trees with maximum Wiener index in $\mathcal{T}^*(n,4)$ are either the tree T_m if $k^2 + k > n-1$, or the tree T'_m if

$k^2+k<n-1$, or the trees T_m and T'_m if $k^2+k=n-1$.

For a tree T in $\mathcal{T}^*(n, n-3)$ with diameter $d=n-3\geq 5$, let P be a path of length $n-3$ in T. Then, there are only two vertices in T, say u and v, that are not on the path P. We partition the trees in $\mathcal{T}^*(n, n-3)$ into two classes: $\mathcal{C}^*(n, n-3)$ and $\overline{\mathcal{C}}^*(n, n-3) = \mathcal{T}^*(n, n-3)\setminus \mathcal{C}^*(n, n-3)$. Then any tree in $\overline{\mathcal{C}}^*(n, n-3)$ must be the tree T^i_{n-3} (for some $2\leq i\leq n-5$) shown in figure 5.

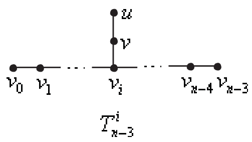


Figure 5: The tree T^i_{n-3} in $\overline{\mathcal{C}}^*(n, n-3)$.

By theorem 2.10, we know that the tree with maximum Wiener index in $\mathcal{C}^*(n, n-3)$ is the tree $D(n, 2, 2)$. By the inverse *i.m.t.*, we can get that the tree with maximum Wiener index in $\overline{\mathcal{C}}^*(n, n-3)$ is the tree T^2_{n-3} (isomorphic to T^{n-5}_{n-3}). Therefore, in order to obtained the tree with maximum Wiener index in $\mathcal{T}^*(n, n-3)$, we only need to compare $W(D(n, 2, 2))$ and $W(T^2_{n-3})$. By formula (1) or (2), we have $W(D(n, 2, 2)) - W(T^2_{n-3}) = 2n-14>0$ for $n-3\geq 5$, and so the tree with maximum Wiener index in $\mathcal{T}^*(n, n-3)$ $(n\geq 8)$ is the tree $D(n, 2, 2)$.

Now, the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$ $(2\leq d\leq 4$ or $5\leq n-3\leq d\leq n-1)$ have all been determined.

For the cases $5\leq d\leq n-4$, it is difficult to characterize the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$. For a fixed value of d and different values of n, the trees with maximum Wiener indices may have different structures. To illustrate this fact, we list the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$ for some values of n and d.

Let $T^i_{n,d}$ $(i=1, 2, \ldots)$ denote the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$. Figure 6 shows the trees with maximum Wiener indices in $\mathcal{T}^*(10, 5)$, $\mathcal{T}^*(10, 6)$, $\mathcal{T}^*(11, 5)$ and $\mathcal{T}^*(11, 6)$, the Wiener indices of which are respectively as follows, $W(T^1_{10,5}) = W(T^2_{10,5}) = 127$, $W(T^1_{10,6}) = 139$, $W(T^1_{11,5}) = W(T^2_{11,5}) = 160$, $W(T^1_{11,6}) = W(T^2_{11,6}) = 176$.

From the above examples, it seems to be impossible to give a universal characterization for the trees with maximum Wiener indices in $\mathcal{T}^*(n, d)$ for $5\leq d\leq n-4$.

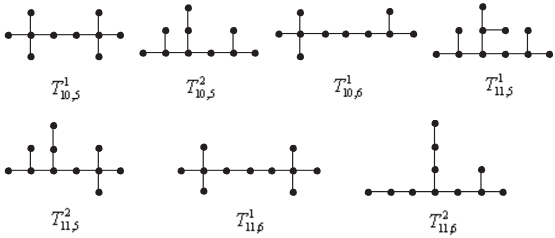


Figure 6: Some trees with maximum Wiener indices in $\mathcal{T}^*(n,d)$, $5 \le d \le n-4$.

3 Wiener index versus maximum degree in trees

In this section, we will characterize the tree with maximum Wiener index in $\mathcal{T}(n,\Delta)$, and the trees with the second and the third maximum Wiener indices in $\mathcal{T}_{1,\Delta}(n)$.

In order to obtain the tree with maximum Wiener index in $\mathcal{T}(n,\Delta)$, we need the following tree transformation, which had been used by Gutman et al. [13].

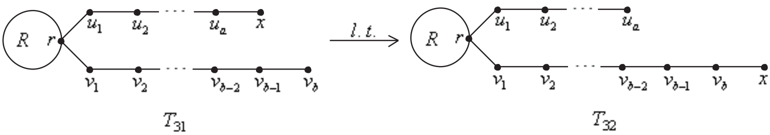


Figure 7: The lengthening transformation of the tree T_{31}.

Let T_{31} and T_{32} be the trees depicted in figure 7, where a and b are two integers satisfying $b > a \ge 0$, and R is a rooted tree with root r and of order greater than 1. For convenience, we call the transformation $T_{31} \to T_{32}$ *the lengthening transformation* of T_{31}, or *the l.t.* of T_{31} for short.

The following lemma is an immediate result of Theorem 2 in Gutman et al. [13].

Lemma 3.1 [13] The lengthening transformation increases the Wiener index, viz.

$$W(T_{31}) < W(T_{32}).$$

Theorem 3.2 If T is a tree in $\mathcal{T}(n,\Delta)$ $(\Delta \ge 3)$, then

$$W(T) \le W(D(n,\Delta-1,1))$$

The equality holds if and only if $T \cong D(n, \Delta - 1, 1)$.

Proof. As $T \in \mathcal{T}(n, \Delta)$, there is at least one vertex, say v, such that $d_T(v) = \Delta$. Viz. there are Δ branches of T at the vertex v. Suppose $T \ncong D(n, \Delta - 1, 1)$. If T is not a starlike tree, then there exist some branches of T at v that are not paths. Then, by repeatedly carrying out the *l.t.* on each of such branches, one can transform T into a starlike tree (say S^*) with v as the unique branching point. If $S^* \ncong D(n, \Delta - 1, 1)$, then S^* can be transformed into $D(n, \Delta - 1, 1)$ by a number of *l.t.* between different branches of S^* at v. By lemma 3.1, $W(T) < W(D(n, \Delta - 1, 1))$. Thus, the result holds. ■

As referred above, Fishermann et al. [6] showed that the tree $C_\Delta(n)$ is the unique tree with maximum Wiener index in $\mathcal{T}_{1,\Delta}(n)$. Now, we define a tree transformation that can be used to obtain the trees with the second and the third maximum Wiener indices in $\mathcal{T}_{1,\Delta}(n)$.

Definition 3.3 Let Δ, a, b be integers satisfying $\Delta \geq 3$, $b > a \geq 0$. And let T_{41} be the tree depicted in figure 8, where T_0 is a rooted tree with root r_0 and $|V(T_0)| > \Delta - 1$. T_{42} is the tree obtained from T_{41} in the following way:
(1)Delete all the edges xx_i $(1 \leq i \leq \Delta - 1)$;
(2)Add all the edges yx_i $(1 \leq i \leq \Delta - 1)$.
The procedures (1) and (2) are called the $(\Delta - 1)$-*regular-lengthening transformation* of T_{41} or $(\Delta - 1)$-*r.l.t.* of T_{41} for short.

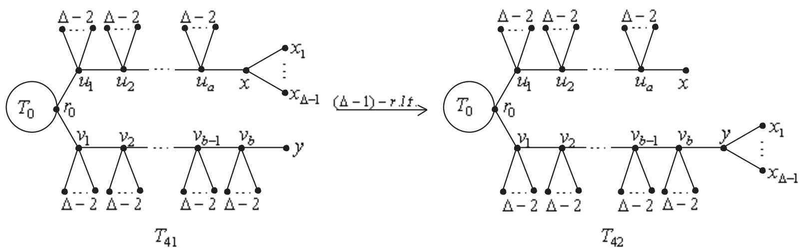


Figure 8: The $(\Delta - 1)$-regular-lengthening transformation of the tree T_{41}.

Lemma 3.4 The $(\Delta - 1)$-*r.l.t.* increases the Wiener index, viz.

$$W(T_{41}) < W(T_{42}).$$

Proof. Let E_1 (resp. E_2) denote the set of all the pendent edges of T_{41} (resp. T_{42}) not in T_0. Then, $|E_1| = |E_2| = (a + b)(\Delta - 2) + \Delta$. Set the paths $P_1^1 = u_1 u_2 \cdots x$ and

$P_1^2 = r_0v_1 \cdots v_b$ in T_{41}. And set $P_2^1 = r_0u_1 \cdots u_a$ and $P_2^2 = v_1v_2 \cdots y$ in T_{42}. Comparing the structures of T_{41} and T_{42}, we can get the following equalities:

$$\sum_{e=uv\in E(T_0)} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv\in E(T_0)} n_u(e|T_{42}) \cdot n_v(e|T_{42});$$

$$\sum_{e=uv\in E_1} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv\in E_2} n_u(e|T_{42}) \cdot n_v(e|T_{42});$$

$$\sum_{e=uv\in E(P_1^1)} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv\in E(P_2^1)} n_u(e|T_{42}) \cdot n_v(e|T_{42});$$

$$\sum_{e=uv\in E(P_1^2)} n_u(e|T_{41}) \cdot n_v(e|T_{41}) = \sum_{e=uv\in E(P_2^2)} n_u(e|T_{42}) \cdot n_v(e|T_{42}).$$

The edges not involved in the above equalities are the edges r_0u_1 in T_{41} and r_0v_1 in T_{42}. Therefore, we have

$$\begin{aligned} &W(T_{42}) - W(T_{41}) \\ &= n_{r_0}(r_0v_1|T_{42}) \cdot n_{v_1}(r_0v_1|T_{42}) - n_{r_0}(r_0u_1|T_{41}) \cdot n_{u_1}(r_0u_1|T_{41}) \\ &= [b(\Delta-1)+\Delta][n-b(\Delta-1)-\Delta] - [a(\Delta-1)+\Delta][n-a(\Delta-1)-\Delta] \\ &= (\Delta-1)(b-a)[n-(a+b)(\Delta-1)-2\Delta] \end{aligned}$$

Note that $|V(T_0)| > \Delta - 1$. $n = |V(T_0)| + (a+b)(\Delta-1) + \Delta + 1 > (\Delta-1) + (a+b)(\Delta-1) + \Delta + 1 = (a+b)(\Delta-1) + 2\Delta$. That is $n - (a+b)(\Delta-1) - 2\Delta > 0$. Furthermore, $\Delta \geq 3$ and $b > a$. So, $W(T_{42}) - W(T_{41}) > 0$, viz. $W(T_{41}) < W(T_{42})$. ■

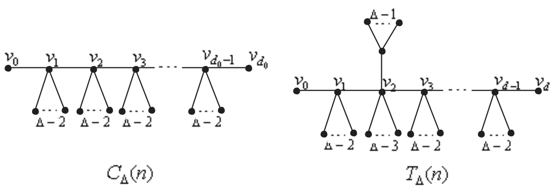


Figure 9: The trees $C_\Delta(n)$ and $T_\Delta(n)$ in $\mathcal{T}_{1,\Delta}(n)$.

From the definition of $C_\Delta(n)$, we can easily get that $C_\Delta(n) \in \mathcal{T}_{1,\Delta}(n)$ is the tree shown in figure 9, where $d_0 = \frac{n-2}{\Delta-1} + 1$. Let $T_\Delta(n) \in \mathcal{T}_{1,\Delta}(n)$ be the tree depicted in figure 9, where $d = d_0 - 1 = \frac{n-2}{\Delta-1} \geq 4$. The following theorem gives the tree with the second maximum Wiener index in $\mathcal{T}_{1,\Delta}(n)$.

Theorem 3.5 If T is a tree in $\mathcal{T}_{1,\Delta}(n) \setminus \{C_\Delta(n), T_\Delta(n)\}$ ($\Delta \geq 3$, $n \geq 4\Delta - 2$), then

$$W(T) < W(T_\Delta(n)) < W(C_\Delta(n)).$$

Proof. Note that $T \neq C_\Delta(n)$ and $T \neq T_\Delta(n)$. By a number of $(\Delta-1)$-*r.l.t.*, T can be transformed into the tree $T_\Delta(n)$. By lemma 3.4, $W(T) < W(T_\Delta(n))$. Furthermore, $T_\Delta(n)$ can be transformed into $C_\Delta(n)$ by a step of $(\Delta-1)$-*r.l.t.*. So by lemma 3.4, $W(T_\Delta(n)) < W(C_\Delta(n))$. Therefore, the result holds. ■

Let $T'_\Delta(n), T''_\Delta(n) \in \mathcal{T}_{1,\Delta}(n)$ be the trees depicted in figure 10, where $d = \frac{n-2}{\Delta-1} \geq 6$. The following theorem presents the tree with the third maximum Wiener index in $\mathcal{T}_{1,\Delta}(n)$.

Theorem 3.6 If T is a tree in $\mathcal{T}_{1,\Delta}(n) \setminus \{C_\Delta(n), T_\Delta(n)\}$ $(\Delta \geq 3,\ n \geq 6\Delta - 4)$, then $W(T) \leq W(T'_\Delta(n))$. The equality holds if and only if $T \cong T'_\Delta(n)$.

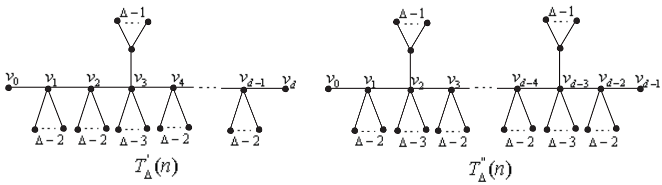


Figure 10: The trees $T'_\Delta(n)$ and $T''_\Delta(n)$ in $\mathcal{T}_{1,\Delta}(n)$.

Proof. Note that $T \in \mathcal{T}_{1,\Delta}(n) \setminus \{C_\Delta(n), T_\Delta(n)\}$. If $T \ncong T'_\Delta(n)$ and $T \ncong T''_\Delta(n)$, then T can be transformed into $T'_\Delta(n)$ by a number of $(\Delta-1)-r.l.t.$. By lemma 3.4, $W(T) < W(T'_\Delta(n))$.

Let P' (resp. P'') be the $(v_3 - v_{d-4})$-path in $T'_\Delta(n)$ (resp. $T''_\Delta(n)$), and let E_1 (resp. E_2) be the set of all the pendent edges of $T'_\Delta(n)$ (resp. $T''_\Delta(n)$). Clearly,
$\sum_{e=uv\in E(P')} n_u(e|T'_\Delta(n)) \cdot n_v(e|T'_\Delta(n)) = \sum_{e=uv\in E(P'')} n_u(e|T''_\Delta(n)) \cdot n_v(e|T''_\Delta(n))$,
$\sum_{e=uv\in E_1} n_u(e|T'_\Delta(n)) \cdot n_v(e|T'_\Delta(n)) = \sum_{e=uv\in E_2} n_u(e|T''_\Delta(n)) \cdot n_v(e|T''_\Delta(n))$.
Comparing the other edges in $T'_\Delta(n)$ and $T''_\Delta(n)$, we have that $W(T'_\Delta(n)) - W(T''_\Delta(n)) = 2(2\Delta-1)[n-(2\Delta-1)] - \Delta(n-\Delta) - (3\Delta-2)[n-(3\Delta-2)] = 2(\Delta-1)^2 > 0$. So $W(T'_\Delta(n)) > W(T''_\Delta(n))$.

Thus, the result holds. ■

It becomes more and more complicated to determine the trees with the $4th, 5th, \ldots,$ maximum Wiener indices in $\mathcal{T}_{1,\Delta}(n)$. Other than the $(\Delta-1)-r.l.t.$, much discussion and comparison are also needed for determining the tree with the $4th$ maximum Wiener index in $\mathcal{T}_{1,\Delta}(n)$. Here, we would not discuss it any more.

References

[1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[2] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[3] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czechoslavak Math. J.* **26** (1976) 283–296.

[4] D. Bonchev, N. Trinajstić, Information theory, distance matrix, and molecular branching, *J. Chem. Phys.* **67** (1977) 4517–4533.

[5] S. C. Liu, L. D. Tong, Y. Yeh, Trees with the minimum Wiener number, *Int. J. Quantum Chem.* **78** (2000) 331–340.

[6] M. Fishermann, A. Hoffmann, D. Rautenbach, L. Székely, L. Volkmann, Wiener index versus maximum degree in trees, *Disc. Appl. Math.* **122** (2002) 127–137.

[7] F. Jelen, E. Triesch, Superdominance order and distance of trees with bounded maximum degree, *Disc. Appl. Math.* **125** (2003) 225–233.

[8] R. Shi, The average distance of trees, *Systems Sci. Math. Sci.* **6** (1993) 18–24.

[9] R. C. Entringer, Bounds for the average distance-inverse degree product in trees, in Y. Alavi, D. R. Lick and A. J. Schwenk (eds), *Combinatorics, Graph Theory, and Algorithms*, New Issues Press, Kalamazoo, 1999, pp. 335–352.

[10] K. Burns and R. C. Entringer, A graph-theoretic view of the United States postal service, in Y. Alavi and A. J. Schwenk (eds), *Graph Theory, Combinatorics and Algorithms: Proceedings of the Seventh International Conference on the Theory and Applications of Graphs*, Wiley, New York, 1995, pp. 323–334.

[11] J. Plesnik, On the sum of all distances in a graph or digraph, *J. Graph Theory* **8** (1984) 1–21.

[12] H. Dong, X. Guo, Ordering trees by their Wiener indices, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 527–540.

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

[14] S. G. Wagner, A class of trees and its Wiener index, *Acta Appl. Math.* **91** (2006) 119–132.