

REVERSE WIENER INDICES OF CONNECTED GRAPHS

Xiaochun Cai and Bo Zhou

*Department of Mathematics, South China Normal University,
Guangzhou 510631, P. R. China
e-mail: zhoubo@scnu.edu.cn*

(Received September 20, 2007)

Abstract

We provide upper and lower bounds on the reverse Wiener index for connected graphs with given numbers of vertices, edges and diameter, and determine respectively the n -vertex trees of fixed number of pendent vertices, the n -vertex trees of fixed maximum degree, the n -vertex trees of fixed matching number, and the n -vertex trees of a given bipartition with greatest reverse Wiener indices. We also consider the Nordhaus–Gaddum–type result for the reverse Wiener index.

1. INTRODUCTION

We consider simple graphs. The Wiener index $W(G)$ of a connected graph G is the sum of distances between all unordered pairs of vertices of G [1]. It is one of the most thoroughly studied molecular–graph–based structure–descriptors, see, e.g., [2, 3, 4]. Its mathematical properties and its use in the structure–property–activity

modeling can be found in [5–11]. However, its degeneracy and low discriminating power have resulted in lack of unambiguity and uniqueness in its properties [12].

With the aim to overcome the shortcomings of Wiener index, a number of mathematical chemists have come up with the modifications, extensions and variants of this index. Randić *et al.* [13] introduced a novel Wiener matrix, for its potential utilization in structure–property studies. Gutman *et al.* [14] introduced a multiplicative version of Wiener index, $\pi(G)$, which is equal to the product of distances between all pairs of vertices of G , and it has also been reported that in the case of alkanes, π and W are highly correlated. Ivanciuc *et al.* [15] introduced Wiener index extension by counting even/odd graph distances. Balaban *et al.* [16] proposed a novel structure–descriptor, the reverse Wiener index.

Let G be a connected graph with n vertices. Then the reverse Wiener index of G is defined as [16]

$$\Lambda = \Lambda(G) = \frac{1}{2}n(n-1)d - W(G)$$

where d is the diameter of G . In [16], general formulae for Λ were presented for several classes of graphs, including complete graph, star, path, cycle and linear polyacenes, relationships between Λ and other structure–descriptors, especially Wiener index, were discussed, and QSPR investigations demonstrated the usefulness of this index. Ivanciuc *et al.* [17] have shown that Λ is able to produce fair QSPR models for standard Gibbs energy of formation and refractive index for $C_6 - C_{10}$ alkanes.

Let P_n and S_n be respectively the n -vertex path and n -vertex star. Let T be a tree with $n > 4$ vertices, different from S_n and P_n . Zhang and Zhou [18] reported that $\Lambda(S_n) < \Lambda(T) < \Lambda(P_n)$. Thus the reverse Wiener index can be used as a branching index.

In this paper, we establish some further properties of the reverse Wiener index of a connected graph. We provide upper and lower bounds on the reverse Wiener index for connected graphs with given numbers of vertices, edges and diameter. Moreover we characterize trees that have maximum reverse Wiener index within some classes of trees. Besides the number of vertices, these classes are specified by the number of pendent vertices, maximum degree, matching number and the numbers of vertices in the bipartition, respectively. We also consider the Nordhaus–Gaddum–type result [19] for the reverse Wiener index.

2. PROPERTIES OF Λ FOR GENERAL GRAPHS

In this section, we present some properties of the reverse Wiener index of a connected graph. A pendent vertex is a vertex of degree one. Let K_n denote the complete graph with n vertices.

Theorem 1. *Let G be a connected graph with $n \geq 2$ vertices, m edges and diameter d . Then*

$$(d-1)m \leq \Lambda(G) \leq \frac{n(n-1)}{2}(d-2) + m$$

with either equality if and only if $d \leq 2$.

Proof: Note that

$$m + 2 \left[\frac{n(n-1)}{2} - m \right] \leq W(G) \leq m + d \left[\frac{n(n-1)}{2} - m \right]$$

i.e.,

$$n(n-1) - m \leq W(G) \leq \frac{n(n-1)}{2}d - (d-1)m$$

with either equality if and only if $d \leq 2$. Now the result follows by the definition of $\Lambda(G)$. \square

Let \mathcal{G} be a class of connected graphs with n vertices, in which every graph possesses $f(n)$ edges, where $f(n)$ is a function of n with $n-1 \leq f(n) < \frac{n(n-1)}{2}$. By Theorem 1, for any $G \in \mathcal{G}$, $\Lambda(G) \geq f(n)$ with equality if and only if the diameter of G is 2. In particular, if $f(n) = n-1$, i.e., G is a tree with n vertices, then $\Lambda(G) \geq n-1$ with equality if and only if $G = S_n$, while if $f(n) = n$, i.e., G is a unicyclic graph with n vertices, then for $n \geq 4$, $\Lambda(G) \geq n$ with equality if and only if G is a quadrangle, a pentagon, or the the graph obtained by attaching $n-3$ pendent vertices to a vertex of a triangle.

From [20, Theorem 2], we have

Theorem 2. *Let G be a graph with n vertices and diameter d . Then*

$$\Lambda(G) \leq \frac{n(n-1)d}{2} - \frac{d(d+1)(d+2)}{6} - \frac{n-d-1}{2} \left(n + \left\lfloor \frac{d^2+1}{2} \right\rfloor \right)$$

with equality if and only if there is a vertex v_0 such that the distance layers V_i , where V_i is a subset of the vertex set consisting of the vertices that are at distance i from v_0 for $i = 0, 1, \dots, d$, fulfill the condition that the subgraphs induced $V_{i-1} \cup V_i$ are complete whenever $1 \leq i \leq d$ and all noncentral layers are trivial.

Corollary 3. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$0 \leq \Lambda(G) \leq \frac{n(n-1)(n-2)}{3}$$

with left equality if and only if $G = K_n$, and with right equality if and only if $G = P_n$.

Proof. Let m and d be respectively the number of edges and the diameter of G . Note that $d \geq 1$ with equality if and only if $G = K_n$. By Theorem 1, $\Lambda(G) \geq 0$ with equality if and only if $G = K_n$.

Let

$$F(n, d) = \frac{n(n-1)d}{2} - \frac{d(d+1)(d+2)}{6} - \frac{n-d-1}{2} \left(n + \left\lfloor \frac{d^2+1}{2} \right\rfloor \right),$$

where $1 \leq d \leq n-1$. If $d = n-1$, then $G = P_n$ and so $\Lambda(G) = \frac{n(n-1)(n-2)}{3}$. Suppose that $1 \leq d \leq n-2$. If d is even, then

$$F(n, d+1) - F(n, d) = \frac{n(n-d)}{2} + \frac{d^2}{4} - \frac{n}{2} > 0.$$

If d is odd, then

$$F(n, d+1) - F(n, d) = \frac{n(n-d)}{2} - \frac{3}{4} + \frac{d^2}{4} - \frac{d}{2} > 0.$$

In either case, we have $F(n, d) < F(n, d+1)$. Now by Theorem 2, we have

$$\Lambda(G) \leq F(n, d) < F(n, d+1) \leq \dots \leq F(n, n-1) = \Lambda(P_n).$$

Thus $\Lambda(G) \leq \Lambda(P_n)$ with equality if and only if $G = P_n$. \square

Corollary 4. *Let G be a connected bipartite graph with $n \geq 3$ vertices. Then*

$$n-1 \leq \Lambda(G) \leq \frac{n(n-1)(n-2)}{3}$$

with left equality if and only if $G = S_n$, and with right equality if and only if $G = P_n$.

Proof. Let m and d be respectively the number of edges and the diameter of G . Note that $d \geq 2$ and $m \geq n-1$ with both equalities if and only if $G = S_n$. Now the result follows from Theorem 1 and Corollary 3. \square

3. PROPERTIES OF Λ FOR TREES

Recall that a caterpillar is a tree in which removal of all pendent vertices gives a path. Let $P_{n,d,i}$ be the caterpillar obtained from the path P_{d+1} labelled as v_0, v_1, \dots, v_d by attaching $n-d-1$ pendent vertices labelled consecutively as v_{d+1}, \dots, v_{n-1} to the vertex v_i of the path, where $3 \leq d \leq n-2$ (see Fig. 1). Clearly, $P_{n,d,i}$ has diameter d for any $1 \leq i \leq d-1$.

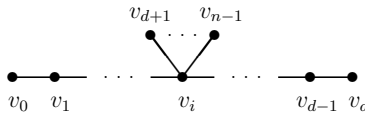


Fig. 1. The graph $P_{n,d,i}$.

Lemma 5. [18] *Let T be a tree with n vertices and diameter d , where $3 \leq d \leq n-2$. If $T \neq P_{n,d,\lfloor \frac{d}{2} \rfloor}$, then $\Lambda(T) < \Lambda(P_{n,d,\lfloor \frac{d}{2} \rfloor})$.*

Lemma 6. [18] *For $3 \leq d \leq n-3$, $\Lambda(P_{n,d,\lfloor \frac{d}{2} \rfloor}) < \Lambda(P_{n,d+1,\lfloor \frac{d+1}{2} \rfloor})$.*

Let T be a tree with n vertices, p of which are pendent vertices, where $2 \leq p \leq n-1$. Obviously, if $p = 2$ then $T = P_n$, and if $p = n-1$ then $T = S_n$. So we can assume that $3 \leq p \leq n-2$.

Theorem 7. *Let T be a tree with n vertices, p of which are pendent vertices, where $3 \leq p \leq n-2$. Then $\Lambda(T) \leq \Lambda(P_{n,n-p+1,\lfloor \frac{n-p+1}{2} \rfloor})$ with equality if and only if $T = P_{n,n-p+1,\lfloor \frac{n-p+1}{2} \rfloor}$.*

Proof. Let d be the diameter of T . It is easy to see that $d \leq n-p+1$. If $d \leq n-p$, then by Lemmas 5 and 6, $\Lambda(T) \leq \Lambda(P_{n,d,\lfloor \frac{d}{2} \rfloor}) \leq \Lambda(P_{n,n-p,\lfloor \frac{n-p}{2} \rfloor}) < \Lambda(P_{n,n-p+1,\lfloor \frac{n-p+1}{2} \rfloor})$. If $d = n-p+1$ and $T \neq P_{n,n-p+1,\lfloor \frac{n-p+1}{2} \rfloor}$, then by Lemma 5, $\Lambda(T) < \Lambda(P_{n,n-p+1,\lfloor \frac{n-p+1}{2} \rfloor})$. Thus the result follows. \square

Let T be a tree with maximum degree Δ , where $2 \leq \Delta \leq n-1$. Obviously, if $\Delta = 2$ then $T = P_n$, and if $\Delta = n-1$ then $T = S_n$. So we can assume that $3 \leq \Delta \leq n-2$. Note that the diameter is at most $n-\Delta+1$. Similar to the proof of Theorem 7, we have

Theorem 8. *Let T be a tree with maximum degree Δ , where $3 \leq \Delta \leq n-2$. Then $\Lambda(T) \leq \Lambda(P_{n,n-\Delta+1,\lfloor \frac{n-\Delta+1}{2} \rfloor})$ with equality if and only if $T = P_{n,n-\Delta+1,\lfloor \frac{n-\Delta+1}{2} \rfloor}$.*

If T is a tree with $n \geq 2$ vertices, then $[1, 2] W(T) = \sum_{e \in E(T)} W(e, T)$, where $E(T)$ is the edge set of T , $W(e, T) = n_{T,1}(e) \cdot n_{T,2}(e)$, $n_{T,1}(e)$ and $n_{T,2}(e)$ are the respectively numbers of vertices of T lying on the two sides of the edge e . We will use this fact in the proof of Lemmas 9 and 11.

A matching is a set of pairwise non-adjacent edges. A maximum matching is a matching that contains the largest possible number of edges. The matching number of a graph G is the size of a maximum matching, denoted by $\beta(G)$.

Let T be a tree with n vertices and matching number k , where $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$. If $k = 1$, then $T = S_n$. So we can assume that $k \geq 2$.

Lemma 9. *For even k with $2 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$, $\Lambda(P_{n,2k-1,k-1}) < \Lambda(P_{n,2k,k-1})$.*

Proof. Note that

$$\Lambda(P_{n,2k,k-1}) - \Lambda(P_{n,2k-1,k-1})$$

$$\begin{aligned}
 &= \frac{n(n-1)}{2} - W(v_{k-1}v_k, P_{n,2k,k-1}) + W(v_{k-1}v_{n-1}, P_{n,2k-1,k-1}) \\
 &\geq \frac{n(n-1)}{2} - \frac{n^2}{4} + W(v_{k-1}v_{n-1}, P_{n,2k-1,k-1}) > 0.
 \end{aligned}$$

The result follows. \square

Lemma 10. *For $2 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$, $\beta(P_{n,2k,k}) = k$ if k is odd, and $\beta(P_{n,2k,k-1}) = k$ if k is even.*

For a tree T with at least two vertices and $u \in V(T)$, d_u denotes the degree of u in T . There are d_u components in $T - u$, each containing a neighbor of u in T . These components are called the branches of T at u .

Lemma 11. *Let T be a tree with n vertices and matching number k , where k is even, $2 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$, and $T \neq P_{n,2k,k-1}$. If the diameter of T is $2k$, then $\Lambda(T) < \Lambda(P_{n,2k,k-1})$.*

Proof. Let $P(T) = v_0v_1 \cdots v_d$ be a diametrical path of T , where $d = 2k$. There is a matching of size k in $P(T)$. So T is a caterpillar.

If there exists an even i_0 , $2 \leq i_0 \leq d - 2$, such that $d_{v_{i_0}} \geq 3$, then $v_{i_0}w \in E(T)$ for some w outside $P(T)$, and so there is a matching of T containing the edge $v_{i_0}w$ of size $1 + \frac{i_0}{2} + \frac{d-i_0}{2} = k + 1$, a contradiction. Hence $d_{v_i} = 2$ for all even i with $2 \leq i \leq d - 2$.

Suppose that there are two vertices v_i, v_j of degree at least three such that the distance between v_i and v_j is as small as possible, where i and j are odd with $1 \leq i < j \leq d - 1$. Then the vertices v_{i+1}, \dots, v_{j-1} have equal degree two. Let n_1 (resp. n_2) be the number of vertices of the branch at v_{i+1} (resp. v_{j-1}) containing v_i (resp. v_j). Then $n_1 + n_2 + (j - i - 1) = n$. Assume that $n_1 \geq n_2$. Let w be a pendent vertex adjacent to v_j . Let T' denote the tree formed from T by deleting edge v_jw and adding edge v_iw . It is easy to see that

$$\begin{aligned}
 \Lambda(T') - \Lambda(T) &= W(T) - W(T') \\
 &= W(v_i v_{i+1}, T) - W(v_{j-1} v_j, T') \\
 &= n_1(n - n_1) - (n_2 - 1)(n - n_2 + 1).
 \end{aligned}$$

Since $n_2 - 1 < \min\{n_1, n - n_1\}$, we have $\Lambda(T') > \Lambda(T)$. By iterating the transformation from T to T' , we have $\Lambda(T) < \Lambda(P_{n,2k,i})$ for some odd i with $1 \leq i \leq 2k - 1$.

Now suppose that $T = P_{n,2k,i}$ for some odd i with $1 \leq i \leq 2k - 1$. Since $T \neq P_{n,2k,k-1}$, we may assume that $1 \leq i \leq k - 3$. It is easy to see that

$$\Lambda(P_{n,2k,i+2}) - \Lambda(P_{n,2k,i})$$

$$\begin{aligned}
&= W(v_i v_{i+1}, P_{n,2k,i}) - W(v_i v_{i+1}, P_{n,2k,i+2}) \\
&\quad + W(v_{i+1} v_{i+2}, P_{n,2k,i}) - W(v_{i+1} v_{i+2}, P_{n,2k,i+2}) \\
&= [(n-2k+i)(2k-i) - (i+1)(n-i-1)] \\
&\quad + [(n-2k+i+1)(2k-i-1) - (i+2)(n-i-2)] .
\end{aligned}$$

Since $i+1 < \min\{n-2k+i, 2k-i\}$ and $i+2 < \min\{n-2k+i+1, 2k-i-1\}$, we have $\Lambda(P_{n,2k,i+2}) > \Lambda(P_{n,k,i})$. Iterating the procedure, we prove the lemma. \square

Theorem 12. *Let T be a tree with n vertices and matching number k , where $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$.*

- (i) *If $k = \lfloor \frac{n}{2} \rfloor$, then $\Lambda(T) \leq \Lambda(P_n)$ with equality if and only if $T = P_n$.*
- (ii) *If $k \leq \lfloor \frac{n}{2} \rfloor - 1$ and k is odd, then $\Lambda(T) \leq \Lambda(P_{n,2k,k})$ with equality if and only if $T = P_{n,2k,k}$.*
- (iii) *If $k \leq \lfloor \frac{n}{2} \rfloor - 1$ and k is even, then $\Lambda(T) \leq \Lambda(P_{n,2k,k-1})$ with equality if and only if $T = P_{n,2k,k-1}$.*

Proof. Note that $\Lambda(T) < \Lambda(P_n)$ for any n -vertex tree different from P_n and that $\beta(P_n) = \lfloor \frac{n}{2} \rfloor$. Hence (i) follows easily.

Suppose that $k \leq \lfloor \frac{n}{2} \rfloor - 1$. Let d be the diameter of T . Obviously, $k \geq \lfloor \frac{d+1}{2} \rfloor$, i.e., $d \leq 2k$.

Suppose that k is odd. If $d \leq 2k-1$, then by Lemmas 5 and 6, we have $\Lambda(T) \leq \Lambda(P_{n,d,\lfloor \frac{d}{2} \rfloor}) \leq \Lambda(P_{n,2k-1,k-1}) < \Lambda(P_{n,2k,k})$. If $d = 2k$ and $T \neq P_{n,2k,k}$, then by Lemma 5, $\Lambda(T) < \Lambda(P_{n,2k,k})$. Furthermore, by Lemma 10, we have $\beta(P_{n,2k,k}) = k$. Hence (ii) follows.

Now suppose that k is even. If $d \leq 2k-1$, then by Lemmas 5, 6 and 9, we have $\Lambda(T) \leq \Lambda(P_{n,d,\lfloor \frac{d}{2} \rfloor}) \leq \Lambda(P_{n,2k-1,k-1}) < \Lambda(P_{n,2k,k-1})$. If $d = 2k$ and $T \neq P_{n,2k,k-1}$, then by Lemma 11, $\Lambda(T) < \Lambda(P_{n,2k,k-1})$. Furthermore, by Lemma 10, we have $\beta(P_{n,2k,k-1}) = k$. Hence (iii) follows. \square

The vertex set of a connected bipartite graph G with at least two vertices can be uniquely partitioned into two disjoint sets V_1 and V_2 such that all edges join a vertex in V_1 to a vertex in V_2 . In this case we say that G has a $(|V_1|, |V_2|)$ -bipartition.

Let T be a tree with an $(s, n-s)$ -bipartition, where $1 \leq s \leq \lfloor \frac{n}{2} \rfloor$. If $s = 1$, then $T = S_n$. So we can assume that $s \geq 2$. Note that P_n has the bipartition $(\lfloor \frac{n}{2} \rfloor, n - \lfloor \frac{n}{2} \rfloor)$ and that the diameter of T is at most $2s$ if $s \leq \lfloor \frac{n}{2} \rfloor - 1$. Similar to the proof of Theorem 12, we have

Theorem 13. *Let T be a tree with an $(s, n - s)$ -bipartition, where $2 \leq s \leq \lfloor \frac{n}{2} \rfloor$.*

- (i) *If $s = \lfloor \frac{n}{2} \rfloor$, then $\Lambda(T) \leq \Lambda(P_n)$ with equality if and only if $T = P_n$.*
- (ii) *If $s \leq \lfloor \frac{n}{2} \rfloor - 1$ and s is odd, then $\Lambda(T) \leq \Lambda(P_{n,2s,s})$ with equality if and only if $T = P_{n,2s,s}$.*
- (iii) *If $s \leq \lfloor \frac{n}{2} \rfloor - 1$ and s is even, then $\Lambda(T) \leq \Lambda(P_{n,2s,s-1})$ with equality if and only if $T = P_{n,2s,s-1}$.*

4. THE NORDHAUS–GADDUM–TYPE RESULT FOR Λ

Nordhaus and Gaddum [19] reported bounds for the chromatic numbers of a graph and its complement. Eventually, Nordhaus–Gaddum–type relations were established for many other graph invariants, see, e.g., [21]. Now we are ready to give bounds of this kind for the reverse Wiener index.

For simplicity, let $m(G)$ and $d(G)$ be respectively the number of edges and the diameter of the graph G .

Lemma 14. *Let G be a graph with $n \geq 6$ vertices. If $d(G) = d(\overline{G}) = 3$, then $\Lambda(G) + \Lambda(\overline{G}) < \frac{(n-1)(n-2)(2n+3)}{6}$.*

Proof. Since $d(G) = d(\overline{G}) = 3$, we have $W(G) + W(\overline{G}) > m(G) + 2m(\overline{G}) + m(\overline{G}) + 2m(G) = \frac{3}{2}n(n-1)$. Thus

$$\begin{aligned} \Lambda(G) + \Lambda(\overline{G}) &= \frac{1}{2}n(n-1) \cdot 6 - [W(G) + W(\overline{G})] \\ &< 3n(n-1) - \frac{3}{2}n(n-1) \\ &= \frac{3}{2}n(n-1) < \frac{(n-1)(n-2)(2n+3)}{6}. \end{aligned}$$

The last inequality holds because $n \geq 6$. \square

Lemma 15. *Let G be a graph of order $n \geq 5$. If $d(\overline{G}) = 2$, then $\Lambda(G) + \Lambda(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$ with equality if and only if $G \cong P_n$.*

Proof. Let $d = d(G)$. By Corollary 2, $\Lambda(G) \leq \Lambda(P_n)$ with equality if and only if $G = P_n$.

Since $n \geq 5$, we have $d(\overline{G}) = d(\overline{P_n}) = 2$, and so $\Lambda(\overline{G}) = m(\overline{G}) \leq \frac{n(n-1)}{2} - (n-1) = m(\overline{P_n}) = \Lambda(\overline{P_n})$ with equality if and only if G is a tree whose complement has diameter

2. Note that

$$\begin{aligned}\Lambda(P_n) + \Lambda(\overline{P_n}) &= \frac{n(n-1)(n-2)}{3} + \frac{n(n-1)}{2} - (n-1) \\ &= \frac{(n-1)(n-2)(2n+3)}{6}.\end{aligned}$$

The result follows easily. \square

Remark. (i) There is exactly one pair of connected graphs G and \overline{G} with 4 vertices: P_4 and $\overline{P_4} = P_4$. Obviously, $d(P_4) = 3$ and $\Lambda(P_4) + \Lambda(\overline{P_4}) = 16$.

(ii) There are exactly five pair of connected graphs G and \overline{G} with 5 vertices, in which three pairs satisfy $d(G) = d(\overline{G}) = 3$: T and \overline{T} , U_1 and $\overline{U_1}$, U_2 and $\overline{U_2} = U_2$, where T be the unique tree with 5 vertices and diameter 3, U_1 is the graph formed from T by adding an edge between its two pendent vertices with a common end vertex, and U_2 is formed from the path P_5 by adding an edge between the two neighbors of its center. The values of $\Lambda(G) + \Lambda(\overline{G})$ for them are respectively 27, 27 and 28. The two other pairs are P_5 and $\overline{P_5}$, C_5 and $\overline{C_5} = C_5$. Note that $\Lambda(P_5) + \Lambda(\overline{P_5}) = 26$.

Theorem 16. *Let G be a graph on $n \geq 6$ vertices with a connected \overline{G} . Then*

$$\frac{1}{2}n(n-1) \leq \Lambda(G) + \Lambda(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$$

with left equality if and only if G and \overline{G} have equal diameter 2 and with right equality if and only if $G = P_n$ or $\overline{P_n}$.

Proof. By Theorem 1,

$$\Lambda(G) + \Lambda(\overline{G}) \geq m(G) + m(\overline{G}) = \frac{1}{2}n(n-1)$$

with equality if and only if G and \overline{G} have equal diameter 2.

If $d(G) = d(\overline{G}) = 3$, and by Lemma 14, we have $\Lambda(G) + \Lambda(\overline{G}) < \frac{(n-1)(n-2)(2n+3)}{6}$.

If $d(\overline{G})=2$, then by Lemma 15, we have $\Lambda(G) + \Lambda(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$ with equality if and only if $G = P_n$. Similarly, if $d(G) = 2$, then $\Lambda(G) + \Lambda(\overline{G}) \leq \frac{(n-1)(n-2)(2n+3)}{6}$ with equality if and only if $G = \overline{P_n}$.

Note that if $d(\overline{G}) \geq 3$ then $d(G) \leq 3$. The result follows. \square

5. CONCLUSIONS

The Wiener index is a well-known measure of graph or network structures with similarly useful variant of the reverse Wiener index. In this paper, we establish some properties of the reverse Wiener index of a connected graph. In particular, we

provide (in Theorems 1 and 2) upper and lower bounds on the reverse Wiener index for connected graphs with given numbers of vertices, edges and diameter, we show (in Theorems 7, 8, 12 and 13) that $P_{n,n-p+1,\lfloor \frac{n-p+1}{2} \rfloor}$ is the unique tree with the greatest reverse Wiener index in the class of n -vertex trees with p pendent vertices or with maximum degree p , where $3 \leq p \leq n-2$, and P_n for $k = \lfloor \frac{n}{2} \rfloor$, $P_{n,2k,k}$ for odd k with $2 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$ and $P_{n,2k,k-1}$ for even k with $2 \leq k \leq \lfloor \frac{n}{2} \rfloor - 1$ is the unique tree with the greatest reverse Wiener index in the class of n -vertex trees with matching number k or with a $(k, n-k)$ -bipartition, where $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$ and we also give (in Theorem 16) the Nordhaus–Gaddum-type result for the reverse Wiener index.

Acknowledgement. This work was supported by the National Natural Science Foundation of China (No. 10671076).

References

- [1] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [2] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.
- [3] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.
- [4] D. H. Rouvray, The rich legacy of half a century of the Wiener index, in: *Topology in Chemistry – Discrete Mathematics of Molecules* (Eds. D. H. Rouvray, R. B. King), Horwood, Chichester, 2002, pp. 16–37.
- [5] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.
- [6] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.
- [7] D. E. Needham, I. C. Wei, P. G. Seybold, Molecular modeling of physical properties of alkanes, *J. Am. Chem. Soc.* **110** (1988) 4186–4194.
- [8] Z. Mihalić, N. Trinajstić, A graph-theoretical approach to structure–property relationships, *J. Chem. Educ.* **69** (1992) 701–712.

- [9] G. Rücker, C. Rücker, On topological indices, boiling points, and cycloalkanes, *J. Chem. Inf. Comput. Sci.* **39** (1999) 788–802.
- [10] S. Nikolić, N. Raos, Estimation of stability constants of mixed amino acid complexes with copper(II) from topological indices, *Croat. Chem. Acta* **74** (2001) 621–631.
- [11] N. Raos, Suitability of the topological index $W^{1/3}$ for estimation of the stability constants of coordination compounds, *Croat. Chem. Acta* **75** (2002) 117–120.
- [12] P. J. Hansen, P. C. Jurs, Chemical applications of graph theory. Part I. Fundamentals and topological indices, *J. Chem. Educ.* **65** (1988) 574–580.
- [13] M. Randić, X. Guo, T. Oxley, H. Krishnapriyan, Wiener matrix: source of novel graph invariants, *J. Chem. Inf. Comput. Sci.* **33** (1993) 709–716.
- [14] I. Gutman, W. Linert, I. Lukovits, Ž. Tomović, The multiplicative version of the Wiener index, *J. Chem. Inf. Comput. Sci.* **40** (2000) 113–116.
- [15] O. Ivanciuc, T. Ivanciuc, D. J. Klein, W. A. Seitz, A. T. Balaban, Wiener index extension by counting even/odd graph distances, *J. Chem. Inf. Comput. Sci.* **41** (2001) 536–549.
- [16] A. T. Balaban, D. Mills, O. Ivanciuc, S. C. Basak, Reverse Wiener indices, *Croat. Chem. Acta* **73** (2000) 923–941.
- [17] O. Ivanciuc, T. Ivanciuc, A. T. Balaban, Quantitative structure–property relationship evaluation of structural descriptors derived from the distance and reverse Wiener matrices, *Internet Electron. J. Mol. Des.* **1** (2002) 467–487.
- [18] B. Zhang, B. Zhou, Modified and reverse Wiener indices of trees, *Z. Naturforsch.* **61a** (2006) 536–540.
- [19] E. A. Nordhaus, J. W. Gaddum, On complementary graphs, *Amer. Math. Monthly* **63** (1956) 175–177.
- [20] J. Plesník, On the sum of all distances in a graph or digraph, *J. Graph Theory* **8** (1984) 1–21.
- [21] L. Zhang, B. Wu, The Nordhaus–Gaddum–type inequalities for some chemical indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 189–194.