MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **69** (2013) 141-150

ISSN 0340 - 6253

On the Wiener and Terminal Wiener Index of Generalized Bethe Trees

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(Received May 6, 2010)

Abstract. Let G be a simple connected graph. The Wiener index of G is equal to the sum of distances between all pairs of vertices of G and terminal Wiener index of G is equal to the sum of distances between all pairs of pendent vertices (vertices of degree one) of G. In this paper we compute the Wiener and terminal Wiener indices of generalized Bethe trees and also for the rooted tree where is obtained by using coalescence of two generalized Bethe trees at rooted vertices. As a application those topological indices for dendrimer trees is computed.

1 Introduction

Let G be a connected graph and $V(G) = \{v_1, v_2, \ldots, v_n\}$ denote the set of vertices of G. The distance $d_G(u, v)$ between two vertices u and v of G is equal to the length of the shortest path that connects vertices u and v in the graph G. The Wiener index of G [1] is defined as

$$W(G) = \sum_{1 \le i < j \le n} d_G(v_i, v_j).$$

For a survey of results and further bibliography on the chemical applications and the mathematical literature of the Wiener index, see [2]-[8] and the references cited therein.

In a number of recently published articles, the so-called terminal distance matrix [9]-[11] or reduced distance matrix [13] of trees was considered. Let G has k pendent vertices labeled by $v_1, v_2, \ldots v_k$, then its terminal distance matrix is the square matrix of order k whose (i, j)-entry is equal to $d_G(v_i, v_j)$. Terminal distance matrices were used for modeling of amino acid sequences of proteins and of the genetic code and were proposed to serve as a source of novel molecularstructure descriptors [9]-[12].

Gutman et al [14] defined the terminal Wiener index $TW(G)$ of the graph G as the sum of distances between all pairs of pendent vertices of G. So

$$TW(G) = \sum_{1\leq i<j\leq k} d_G(v_i, v_j) \ .$$

Recall that a tree is a connected acyclic graph. In a tree, any vertex can be chosen as the root vertex. The level of a vertex on a tree is one more than its distance from the root vertex. Suppose T is an unweighted rooted tree such that its vertices at the same level have equal degrees. We agree that the root vertex is at level 1 and that T has k levels. In [15], Rojo and Robbiano, called such a tree generalized Bethe tree. They denoted the class of generalized Bethe trees of k levels by B_k.

A dendrimer tree $T_{k,d}$ is a rooted tree such that degree of whose non-pendent vertices is equal to d and distance between the rooted (central) vertex and pendent vertices is equal to k [2]. So $T_{k,d}$ can be considered as a generalized Bethe tree with $k+1$ levels such that whose non-pendent vertices have equal degrees. In this paper we will find exact formulas for Wiener and terminal Wiener indices of generalized Bethe trees and also for the rooted tree where obtained by attaching two generalized Bethe trees at the rooted vertices by using coalescence of two graphs. As application the Wiener and the terminal Wiener indices of dendrimer trees will be computed.

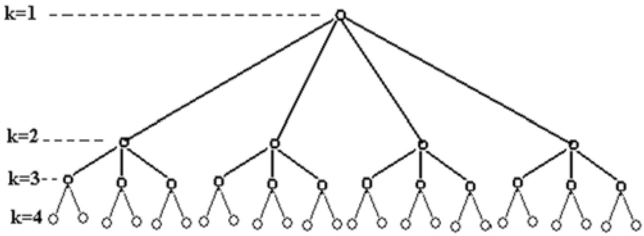

Figure 1: A generalized Bethe tree of 4 levels.

2 Main Results

In this section at first we compute the Wiener index of generalized Bethe trees by using the Wiener's formula. In his seminal article [1] Wiener communicated the formula

$$W(T) = \sum_{e\in E(T)} n_1(e).n_2(e). \tag{1}$$

which holds for any tree T. This result may be viewed as the first theorem ever for the Wiener index. In formula (1), e stands for an edge, whereas $n_1(e)$ and $n_2(e)$ are the number of vertices lying on the two sides of e and the summation goes over all edges of the respective tree T.

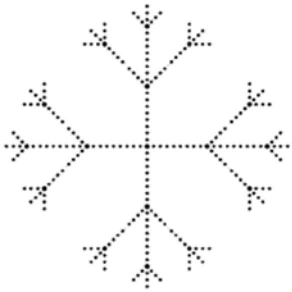

Figure 2: Graph of Dendrimer tree $T_{3,4}$.

Let B_{k+1} be a generalized Bethe tree of $k+1$ levels, degree of whose rooted vertex is equal to d_1 and degree of vertices on the i-th level of B_{k+1} is equal to d_i+1 for $i=2,3,\ldots,k$. So each vertex on the i-th level is adjacent to d_i vertices on the $i+1$-th level of B_{k+1}.

Now suppose that n_i denotes the number of vertices where are located on the i-th level of B_{k+1}. Thus $n_1=1$ and for $i=2,3,\ldots,k+1$, n_i is computed as follows:

$$n_i = d_1 d_2 d_3 \ldots d_{i-1} \; . \tag{2}$$

If n denotes the number of the vertices of B_{k+1}, easy calculation shows that

$$n = n_1 + n_2 + n_3 + \ldots + n_{k+1} = 1 + \sum_{i=1}^{k} \prod_{j=1}^{i} d_j \; . \tag{3}$$

In continue we suppose that $e=uv$ denotes an edge of B_{k+1} where adjacent u on the i-th level and v on the $i+1$-th level of B_{k+1} for $1 \le i \le k$. To compute the Wiener index of B_{k+1}, the number of the vertices lying on the two sides of e must be computed (see fig. 3). Obviously all of the children of vertex v are lying one side of edge $e=uv$ so if m_i denotes the number of those vertices of the tree then $m_k=1$ and

$$m_i = 1 + d_{i+1} + d_{i+1}d_{i+2} + \ldots d_{i+1}d_{i+2}\ldots d_k = 1 + \sum_{j=i+1}^{k} \prod_{r=i+1}^{j} d_r \; . \tag{4}$$

Now we can compute the Wiener index of the generalized Bethe tree of $k+1$ levels in term of degrees of the vertices of this tree.

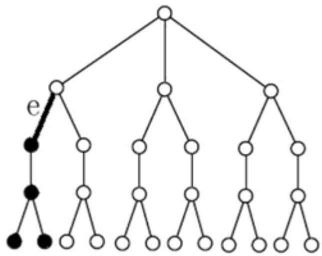

Figure 3: The black and write vertices which lying two sides of edge $e \in E(B_5)$.

Theorem 1. *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:* $W(B_{k+1}) = \sum_{i=1}^{k}(n_{i+1}-1)m_i(n-m_i)$.

Proof. Let e be an edge of B_{k+1} where adjacent a vertex on the i-th level to a vertex on the $i+1$-level of B_{k+1}. The numbers of vertices where lying two sides of e are equal to $n_1(e) = m_i$ and $n_2(e) = n - m_i$. 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 $n_{i+1}-1$, by using (1) we have

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

Therefore proof is completed. ∎

Now we consider dendrimer tree $T_{k,d}$. In this tree degree of the vertices on the i-th level is equal to d for $1 \le i \le k$ and obviously degree of the pendent vertices is equal to 1. In the following Corollary we obtain the exact formula of Wiener index of dendrimer trees where had been obtained by Gutman et al. [14].

Corollary 1. 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

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

Proof. Since degree of the non-pendent vertices of $T_{k,d}$ is equal to d, thus by using (2) the number of vertices on the i-th level of tree is equal to $n_i = d(d-1)^{i-1}$, for $1 < i \leq k+1$ and $n_1 = 1$. So by using (3) and (4) we have

$$\begin{aligned} n &= 1 + \frac{d\left((d-1)^k - 1\right)}{d-2} \\ m_i &= 1 + \frac{(d-1)\left((d-1)^i - 1\right)}{d-2} \ . \end{aligned}$$

So Corollary is proved by replacing the value of n_i, n and m_i form the obtained formula of Theorem 1. ■

In continue we compute the terminal Wiener index of generalized Bethe trees by using a method similar to the method of computation Wiener index of trees which had been obtained by Gutman et al. [14] as follows:

$$TW(T) = \sum_{e \in E(T)} p_1(e).p_2(e) \ . \tag{5}$$

which holds for any tree T . In formula (5) e stands for an edge, whereas $p_1(e)$ and $p_2(e)$ are the number of pendent vertices lying on the two sides of e and the summation goes over all edges of the respective tree T.

Now suppose B_{k+1} is a generalized Bethe tree of $k+1$ levels. The pendent vertices of this tree are located on the last level of tree. If n' denotes the number of pendent vertices of B_{k+1} then

$$n' = d_1 d_2 d_3 \ldots d_k \ . \tag{6}$$

Let $e = uv$ be an edge of B_{k+1} such that adjacent vertex u on the i-th level to vertex v on the $i+1$-th level of B_{k+1} for $1 \leq i \leq k$. If m'_i and m''_i denote the number of pendent vertices of tree where lying on the two sides of e then

$$m'_i = 1 + d_{i+1} d_{i+2} \ldots d_k \ . \tag{7}$$

$$m''_i = n' - 1 - d_{i+1} d_{i+2} \ldots d_k \ . \tag{8}$$

In the following Theorem the terminal Wiener index of generalized Bethe tree will be computed in term of degrees of the vertices of this tree.

Theorem 2. *Let B_{k+1} be a generalized Bethe tree of $k+1$ levels. Then the terminal Wiener index of B_{k+1} is computed as*

$$TW(B_{k+1}) = \prod_{i=1}^{k} d_i + \left(k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{i} d_{k-j+1} \right) \ .$$

Proof. Let e denote one of the $d_1 d_2 \dots d_i$ edges of B_{k+1} such that adjacent a vertex on the i-th level to a vertex on $i+1$-th level of B_{k+1} for $1 \le i \le k$. By using (7) and (8) we have $p_i(e) = 1 + d_{i+1}d_{i+2}\dots d_k$ and $p_2(e) = n' - 1 - d_{i+1}d_{i+2}\dots d_k$. Thus the terminal Wiener index of B_{k+1} is computed as

$$\begin{aligned} WT(B_{k+1}) &= \sum_{e \in E(B_{k+1})} p_1(e).p_2(e) \\ &= \sum_{i=1}^{k} (d_1 d_2 \dots d_i)(1 + d_{i+1}d_{i+2}\dots d_k)(n' - 1 - d_{i+1}d_{i+2}\dots d_k) \\ &= \prod_{i=1}^{k} d_i + \left(k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{i} d_{k-j+1} \right) . \end{aligned}$$

Therefore proof is completed. ■

In the following Corollary we suppose the non-pendent vertices of generalized Bethe tree of $k+1$ levels have equal degree and compute the terminal Wiener index of dendrimer trees.

Corollary 2. 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 terminal Wiener index of $T_{k,d}$ is computed as follows

$$TW(T_{k,d}) = d(d-1)^{2k-2} \left(kd + \frac{(d-1)^{1-k} - d + 1}{d-2} \right) .$$

Proof. Since all of the non-pendent vertices of $T_{k,d}$ have same degree such as d thus $T_{k,d}$ can be considered as generalized Bethe tree of $k+1$ levels such that degree of whose rooted vertex is equal to d and degree of the vertices on the i-th level of tree is equal to $d-1$ for $1 < i < k+1$. By using Theorem 2 we have

$$\begin{aligned} WT(T_{k,d}) &= \prod_{i=1}^{k} d_i + \left(k \prod_{i=1}^{k} d_i - 1 - \sum_{i=1}^{k-1} \prod_{j=1}^{i} d_{k-j-1} \right) \\ &= d \prod_{i=2}^{k} (d-1) + \left(kd \prod_{i=2}^{k} (d-1) - 1 - d(d-1)^{k-2} - \sum_{i=1}^{k-2} \prod_{j=1}^{i} d_{k-j-1} \right) \\ &= d(d-1)^{2k-2} \left(kd + \frac{(d-1)^{1-k} - d + 1}{d-2} \right) . \end{aligned}$$

Therefore proof is completed. ■

Let G and H be two rooted graphs. Recall that the graph which is obtained by identifying the root vertices of G and H is called coalescence of G and H and will be denoted by $G \circ H$. Suppose v denotes the common root vertex of G and H in $G \circ H$ and $d_G(v)$ (or $d_H(v)$) denotes the sum of the distances between v and other vertices of G (or H). The Wiener index of $G \circ H$ was computed as follows [11].

Theorem 3. *Let G and H be n-vertex and m-vertex connected graph respectively. Then the Wiener index of the coalescence of G and H is computed as*

$$W(G \circ H) = W(G) + W(H) + (m-1)d_G(v) + (n-1)d_H(v)\ .$$

Now let $d_G^1(v)$ and $d_H^1(v)$ denote the sum of the distances between the common rooted vertex v and all of the pendent vertices of G and H respectively. Put $\alpha = 0$ if v is a non-pendent vertex of G and H, $\alpha = 1$ if v is a pendent vertex of G or H and at least $\alpha = 2$ if v is pendent vertex of the graphs G and H. In the following Theorem the terminal Wiener index of $G \circ H$ will be computed by using previous notation.

Theorem 4. *Let G and H be rooted trees with n_1 and m_1 pendent vertices respectively. The terminal Wiener index of the coalescence of G and H is computed as*

$$TW(G \circ H) = TW(G) + TW(H) + (m_1 - \alpha)d_G^1(v) + (n_1 - \alpha)d_H^1(v)\ .$$

Proof. Let $\{v_1, v_2, \ldots, v_{n_1}\}$ and $\{u_1, u_2, \ldots, u_{m_1}\}$ denote the pendent vertices of G and H respectively. If v is a nonpendent vertex of G and H then

$$\begin{aligned} WT(G \circ H) &= \sum_{1 \le i < j \le n_1} d_G(v_i, v_j) + \sum_{1 \le i < j \le m_1} d_H(u_i, u_j) + \frac{1}{2}\sum_{i=1}^{n_1}\sum_{j=1}^{m_1} d_{G\circ H}(v_i, u_j) \\ &= TW(G) + TW(H) + \sum_{i=1}^{n_1}\left(d_H^1(v) + m_1 d_G(v_i, v)\right) \\ &= TW(G) + TW(H) + m_1 d_G^1(v) + n_1 d_H^1(v)\ . \end{aligned}$$

If v is a pendent vertex of G or H then without loss generality we suppose that v is pendent vertex of H and a non-pendent vertex of G. So

$$\begin{aligned} WT(G \circ H) &= TW(G) + TW(H) - d_H^1(v) + \sum_{i=1}^{n_1}\left(d_H^1(v) + (m_1 - 1) d_G(v_i, v)\right) \\ &= TW(G) + TW(H) + (m_1 - 1)d_G^1(v) + (n_1 - 1)d_H^1(v)\ . \end{aligned}$$

At least we suppose that v is a pendent vertex of graphs H and G. If $v = v_{n_1}$ then

$$\begin{aligned} WT(G \circ H) &= TW(G) - d_G^1(v) + TW(H) - d_H^1(v) \\ &+ \sum_{i=1}^{n_1-1} \left(d_H^1(v) + (m_1 - 1)d_G(v_i, v)\right) \\ &= TW(G) + TW(H) + (m_1 - 2)d_G^1(v) + (n_1 - 2)d_H^1(v)\ . \end{aligned}$$

Therefore proof is completed. ■

Now let B_{k+1} and B'_{t+1} be two generalized Bethe trees of $k+1$ and $t+1$ levels respectively. If d_i (or d'_i) denote the numbers of vertices on the $i+1$-th level of tree such that are adjacent to a vertex on the i-th level of B_{k+1} (or B'_{t+1}) for $1 \leq i \leq k$ (or $1 \leq i \leq t$) then by using Theorems 3 and 4 the Wiener and terminal Wiener indices of coalescence of two generalized Bethe tree will be computed in the following Corollary.

Corollary 3. Let B_{k+1} and B'_{t+1} be two n-vertex and m-vertex generalized Bethe trees of $k+1$ and $t+1$ levels respectively. The Wiener and terminal Wiener indices of B_{k+1} and B'_{t+1} are computed as

$$W(B_{k+1} \circ B'_{t+1}) = W(B_{k+1}) + W(B'_{t+1}) + (n-1)\sum_{i=1}^{k}\prod_{j=1}^{i} id_j + (m-1)\sum_{i=1}^{t}\prod_{j=1}^{i} id'_j\ .$$

And

$$\begin{aligned} TW(B_{k+1} \circ B'_{t+1}) &= TW(B_{k+1}) + TW(B'_{t+1}) \\ &+ k\left(\prod_{i=1}^{k} d_i - \alpha\right)\left(\prod_{i=1}^{k} d_i\right) + t\left(\prod_{i=1}^{t} d'_i - \alpha\right)\left(\prod_{i=1}^{t} d'_i\right)\ . \end{aligned}$$

Proof. Let v be the rooted vertex B_{k+1} and $d_{B_{k+1}}(v)$ denote the sum of the distances between v and other vertices of B_{k+1}. Then

$$d_{B_{k+1}}(v) = d_1 + 2d_1d_2 + 3d_1d_2d_3 + \ldots + kd_1d_2\cdots d_k = \sum_{i=1}^{k}\prod_{j=1}^{i} id_j\ .$$

By using Theorem 3 we have

$$W(B_{k+1} \circ B'_{t+1}) = W(B_{k+1}) + W(B'_{t+1}) + (n-1)\sum_{i=1}^{k}\prod_{j=1}^{i} id_j + (m-1)\sum_{i=1}^{t}\prod_{j=1}^{i} id'_j\ .$$

Now let $d^1_{B_{k+1}}(v)$ and $d^1_{B'_{t+1}}(v)$ denote the sum of the distances between v and other pendent vertices of B_{k+1} and B'_{t+1} respectively. Then $d^1_{B_{k+1}}(v) = kd_1d_2\cdots d_k$ and

$d^1_{B'_{t+1}}(v) = td'_1 d'_2 \cdots d'_k$. Since the number of the pendent vertices of B_{k+1} and B'_{t+1} are computed as $d_1 d_2 d_3 \ldots d_k$ and $d'_1 d'_2 d'_3 \ldots d'_t$ respectively, by using of Theorem 4 the terminal Wiener index of $B_{k+1} \circ B'_{t+1}$ is computed as follow:

$$\begin{aligned} TW(B_{k+1} \circ B'_{t+1}) &= TW(B_{k+1}) + TW(B'_{t+1}) \\ &+ k\left(\prod_{i=1}^{k} d_i - \alpha\right)\left(\prod_{i=1}^{k} d_i\right) + t\left(\prod_{i=1}^{t} d'_i - \alpha\right)\left(\prod_{i=1}^{t} d'_i\right) . \end{aligned}$$

Therefore proof is completed. ■

Acknowledgement. The Authors would like to thank the anonymous referee for useful comments.

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