International Journal of Engineering, Mathematical and Physical Sciences
ISSN: 2517-9934
Vol:7, No:5, 2013

Terminal Wiener Index for Graph Structures

J. Baskar Babujee and J. Senbagamalar,

Abstract—The topological distance between a pair of vertices i and j, which is denoted by $d(v_i, v_j)$, is the number of edges of the shortest path joining i and j. The Wiener index $W(G)$ is the sum of distances between all pairs of vertices of a graph G. $W(G) = \sum_{i<j} d(v_i, v_j|G)$ where $d(v_i, v_j|G)$ is the distance between the vertices v_i and v_j in a graph. The Terminal Wiener index $TW(G)$ is defined as the sum of the distance between all pairs of pendent vertices in a graph G. In this paper we analyze various types of trees, caterpillar graphs isomorphic to molecular structures and Terminal Wiener index for generalized graphs.

Keywords—Graph, Degree, Distance, Pendent vertex, Wiener index, Tree.

I. Introduction

In order to obtain the structure-activity relationships in which theoretical and computational methods are based it is necessary to find appropriate representations of the molecular structure of chemical compounds. These representations are realized through the molecular descriptors [7]. Molecular descriptors are numbers containing structural information derived from the structural representation used for molecules under study. A molecular graph [6] is a collection of points representing vertices and the lines are named edges in the graph theory language.

In mathematical terms a graph is represented as $G = (V, E)$ where V be the set of vertices and E be the set of edges. Let G be an undirected connected graph without loops or multiple edges with n vertices, denoted by $\{v_1, v_2, v_3, \ldots, v_n\}$. The topological distance between a pair of vertices i and j, which is denoted by $d(v_i, v_j)$, is the number of edges of the shortest path joining i and j. In 1947 Harold Wiener [4] defined the Wiener index $W(G)$ is the sum of distances between all pairs of vertices of a graph G. $W(G) = \sum_{i<j} d(v_i, v_j|G)$ where $d(v_i, v_j|G)$ is the distance between the vertices v_i and v_j in a graph. Among all the trees on n vertices, the star $K_{1,n-1}$ has the lowest Wiener number and the path P_n has the largest Wiener number.

In a number of recent studies, the terminal distance matrix or reduced distance matrix of trees was introduced by Gutman, B. Furtula, and M. Petrovic [5]. If an n-vertex graph G has k pendent vertices (= vertices of degree one), labeled $v_1, v_2, v_3, \ldots, v_k$, then its terminal distance matrix is the square matrix of order k whose (i, j)-entry is $d(v_i, v_j|G)$. The Terminal Wiener index $TW(G)$ of a graph G is the sum of the distances between all pairs of pendent vertices. $TW(G) = \sum_{1\le i<j\le k} d(v_i, v_j|G)$ where $d(v_i, v_j|G)$ is the distance between pair of pendent vertices in a graph G.

Consider a graph G, vertices having degree one is called pendent vertices or terminal vertices and vertices having more than one degree are called interior vertices [2]. In our paper we represent the sum of the distance between all the pair of pendent vertices by $TW(G)$ [1], and sum of the distance between all pair of interior vertices as $IW(G)$. We use the notations the graph K_n^{+k} is obtained from a complete graph K_n by adding a pendent edge to any of the vertex in K_n. The graph G^+ is obtained from any arbitrary graph G by adding a pendent edge to each vertex of G. The graph G^t is obtained from graph G by joining a pendent edge to all the interior vertices of G. The generalized star graph [3] $K_{1,n_1,n_2,\ldots,n_m}$ is obtained by joining one of the pendant vertices of each paths $P_{n_1}, P_{n_2}, \ldots, P_{n_m}$ by an n edge to a common vertex. The $K_{1,n_1,n_2,\ldots,n_m}$ has $n_1 + n_2 + \cdots + n_m + 1$ vertices and $n_1 + n_2 + \cdots + nm$ edges.

J. Baskar Babujee and J. Senbagamalar are with the Department of Mathematics, Anna University, Chennai - 600 025, India e-mail: baskarbabujee@yahoo.com

II. Main Results

Theorem 1: The Terminal Wiener index of full binary tree (FBT) is $2^{l-1} \sum_{m=1}^{l} m2^m$.

Proof: The level of a vertex is the number of edges along the unique path between it and the root. The level of the root is defined as 0. The vertices immediately under the root are said to be in level 1 and so on. A full binary tree is a binary tree in which each internal vertex has exactly two children. If T is full Binary tree with i internal vertices, then T has $i+1$ terminal vertices and $2i+1$ total vertices. The maximum number of vertices on level m in a binary tree is 2^m. We calculate a Terminal Wiener index of full binary tree is
$TW(FBT) = 1.2 + 2.2^2 + 3.2^2 + \cdots +$ upto to m^{th} level
$TW(FBT) = 2^{l-1} \sum_{m=1}^{l} m2^m$, where l is the level of the tree starting from 0^{th} level. ■

Theorem 2: The Terminal Wiener index of the generalized star $K_{1,n_1,n_2,\ldots,n_m}$ is

$$TW(K_{1,n_1,n_2,\ldots,n_m}) = \begin{cases} mn(m-1) & \text{if all } n_i's \text{ are equal} \\ (n_1 + n_2 + \cdots + n_m)(m-1) & \text{if all } n_i's \text{ need not be equal} \end{cases}$$

Proof: Let $K_{1,n_1,n_2,\ldots,n_m}$ be the given star graph with root vertex u. Let be the rooted tree obtained from $K_{1,n_1,n_2,\ldots,n_m}$ by replacing each edge by $\{n_i\}_{i=1}^{m}$ paths.

Case (i): all n_i's are equal

$$TW(K_{1,n_1,n_2,\ldots,n_m})$$
$$= \frac{1}{2}\left\{\underbrace{\underbrace{(2n+2n+\cdots+2n)}_{m\ times}+\cdots+\underbrace{(2n+2n+\cdots+2n)}_{m\ times}}_{m\ times}\right\}$$

$TW(K_{1,n_1,n_2,\ldots,n_m}) = mn(m-1)$

Case (ii): all n_i's need not be equal

$TW(K_{1,n_1,n_2,\ldots,n_m}) = \frac{1}{2}\{((n_1+n_2)+\cdots+(n_1+n_m)) + ((n_2+n_1)+\cdots+(n_2+n_m)) + \cdots + ((n_m+n_1)+\cdots+(n_m+n_{m-1}))\}$

$TW(K_{1,n_1,n_2,\ldots,n_m}) = \frac{1}{2}\{(m-1)(n_2+n_3+\cdots+n_m) + (m-1)(n_1+n_2+\cdots+n_{m-1})\}$

$TW(K_{1,n_1,n_2,\ldots,n_m}) = \frac{1}{2}\{(m-1)(n_1+n_2+\cdots+n_m) + m(n_1+n_2+\cdots+n_m) - (n_1+n_2+\cdots+n_m)\}$

$TW(K_{1,n_1,n_2,\ldots,n_m}) = (m-1)(n_1+n_2+\cdots+n_m)$. ∎

Theorem 3: The Wiener index of K_n^{+k} is $\frac{1}{2}\{n^2+n(4k-1)+k(3k-5)\}$.

Proof: Consider a complete graph $K_n(V,E)$ with n vertices. Let the vertex set be $V = \{v_1,v_2,v_3,\ldots,v_n\}$. Construct a graph K_n^{+k} by adding a pendent vertex for some k vertices of K_n. Let the vertex set of $K_n^{+k}(V',E')$ be $V' = V\cup\{v_1',v_2',v_3',\ldots,v_k'\}$ and edge set be $E' = E\cup(v_1v_1',v_2v_2',\ldots,v_kv_k')$.

$$W(K_n^k) = \frac{1}{2}\left\{k\left(\underbrace{1+1+\cdots+1}_{n-1\ times}\right)\left(\underbrace{2+2+\cdots+2}_{n-1\ times}\right)\right.$$
$$+(n-k)\left\{\left(\underbrace{1+1+\cdots+1}_{n-1\ times}\right)\left(\underbrace{2+2+\cdots+2}_{n-1\ times}\right)\right\}$$
$$\left.+\left\{k\left(1+\left(\underbrace{2+2+\cdots+2}_{n-1\ times}\right)\right)+\left(\underbrace{3+3+\cdots+3}_{k-1\ times}\right)\right\}\right\}$$

$W(K_n^{+k}) = \frac{1}{2}\{n^2+n(4k-1)+k(3k-5)\}$. ∎

Theorem 4: Let G be a graph, with k pendent vertices. By joining a pendent edge to all the pendent vertices successively then the Terminal Wiener index in the p^{th} stage is $TW(G)+pk(k-1)$.

Theorem 5: Let G be a graph with k pendent vertices. If G' be a graph obtained from G by joining m pendent edges to every k pendent vertices, then the Terminal Wiener index of G' is $m^2TW(G)+mk(mk-1)$.

Theorem 6: If G be a graph with n vertices and at least one vertex has degree $n-1$ then $TW(G)=k(k-1)$ where k is the number of pendent vertices in G.

Theorem 7: Let G be a connected graph with n vertices such that there is at least one vertex v with degree $n-1$. The graph G^x obtained by connecting m copies of G by adding m new edges from each v of G to a new vertex x. Then $TW(G^x) = mk[k(2m-1)-1]$ where k is the number of pendent vertices in G.

Proof: By definition

$$TW(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i,v_j|G)$$
$$= \frac{1}{2}\left\{m\left[\left[\left(\underbrace{\underbrace{(2+2+\cdots+2)}_{k-1\ times}+\cdots+\underbrace{2+2+\cdots+2}_{k-1\ times}}_{k\ times}\right)\right.\right.\right.$$
$$\left.\left.\left.+\left(\underbrace{\underbrace{(4+4+\cdots+4)}_{k\ times}+\cdots+\underbrace{4+4+\cdots+4}_{k\ times}}_{m-1\ copies}\right)\right]\right]\right\}$$
$$= \frac{1}{2}\left\{\underbrace{2k(k-1)+\cdots+2k(k-1)}_{m\ copies}\right.$$
$$\left.+(m-1)\underbrace{4k^2+4k^2+\cdots+4k^2}_{m\ copies}\right\}$$
$$= \frac{1}{2}\{2mk(k-1)+4k^2m(m-1)\}$$
$$TW(G) = mk[k(2m-1)-1].$$
∎

Theorem 8: The Wiener index of G^+ is $4W(G)+n(2n-1)$.

Proof: For any arbitrary graph G, let the vertex set be $V = \{v_1,v_2,v_3,\ldots,v_n\}$. Construct a graph G^+ by adding a pendent edge to each vertex of G. Now $G^+(V',E')$ is denoted by G^+ where $V' = V\cup\{v_1',v_2',v_3',\ldots,v_n'\}$, $|V'| = 2n$ and $|E'| = |E|+n$, $E' = E\cup\{v1v1',v2v2',\ldots,vnvn'\}$. Splitting a Wiener index of G^+ into four parts, (i.e.) half sum of the shortest distance between the vertices in G and half sum of the shortest distance between vertices in G to pendent vertices in G^+ and half sum of the shortest distance between pendent vertices in G^+ to vertices in G and half sum of the shortest distance between the pendent vertices in G^+ to pendent vertices in G^+.

$$W(G^+) = \frac{1}{2}\left\{\sum_{v_i,v_j\in V} d(v_i,v_j|G) + \sum_{\substack{v_i\in V\\ v_j'\in V'}} d(v_i,v_j'|G^+)\right.$$
$$\left.+\sum_{\substack{v_j'\in V'\\ v_i\in V}} d(v_j',v_i|G^+) + \sum_{\substack{v_i'\in V'\\ v_i'\in V'}} d(v_i',v_j'|G^+)\right\}$$
$$= \frac{1}{2}\left\{\sum_{v_i,v_j\in V} d(v_i,v_j|G)\right.$$
$$+\left\{\begin{array}{c} d(v_1,v_1')+d(v_1,v_2')+\cdots+d(v_1,v_n') \\ +d(v_2,v_1')+d(v_2,v_2')+\cdots+d(v_2,v_n') \\ +\cdots+\cdots+\cdots+\cdots \\ +d(v_n,v_1')+d(v_n,v_2')+\cdots+d(v_n,v_n') \end{array}\right\}$$

$$+\left\{\begin{array}{c} d(v_1',v_1)+d(v_1',v_2)+\cdots+d(v_1',v_n)\\ +d(v_2',v_1)+d(v_2',v_2)+\cdots+d(v_2',v_n)\\ +\cdots+\cdots+\cdots+\cdots\\ +d(v_n',v_1)+d(v_n',v_2)+\cdots+d(v_n',v_n)\end{array}\right\}$$

$$+\left\{\begin{array}{c} d(v_1',v_1')+d(v_1',v_2')+\cdots+d(v_1',v_n')\\ +d(v_2',v_1')+d(v_2',v_2')+\cdots+d(v_2',v_n')\\ +\cdots+\cdots+\cdots+\cdots\\ +d(v_n',v_1')+d(v_n',v_2')+\cdots+d(v_n',v_n')\end{array}\right\}$$

$$=\frac{1}{2}\{2W(G)+n+n(n-1)+2W(G)$$
$$+n+n(n-1)+2W(G)+2n(n-1)+2W(G)\}$$
$$W(G^+)=4W(G)+n(2n-1).$$

■

Theorem 9: Let $W(G)$ be a Wiener Index of a connected graph G. If G^t is a graph obtained from G by joining exactly one pendent edge to all the n_1 interior vertices of G, then $TW(G^t)=W(G)+n_1(n_1+n_0-1)$ where n_0 is the number of pendent vertices in G.

Proof: Let G be a graph. The vertex set be $\{v_1,v_2,v_3,\ldots,v_{n_0},v_1,v_2,\ldots,v_{n_1}\}$. The vertices $v_1,v_2,v_3,\ldots,v_{n_0}=n_0$ are called terminal vertices of G. The vertices $v_1,v_2,\ldots,v_{n_1}=n_1$ are called interior vertices of G. $k_0+k_1=n$ be the number of vertices of a graph G. The graph G^t is obtained from G by joining a pendent edge to all the interior vertices of $\{v_1,v_2,v_3,\ldots,v_{n_1}\}$. The new pendent vertices be $\{v_1',v_2',v_3',\ldots,v_{n_1}'\}.n_1+n_0+n_1=N$ be the number of vertices of a graph G^t. By definition

$$TW(G^t)=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}d(v_i,v_j|G^t)$$
$$=\frac{1}{2}\left\{\sum_{i=1}^{n_1'}\sum_{j=1}^{n_1'}d(v_i,v_j|G^t)+\sum_{i=1}^{n_1'}\sum_{j=1}^{n_1}d(v_i,v_j|G^t)\right.$$
$$\left.+\sum_{i=1}^{n_1}\sum_{j=1}^{n_1'}d(v_i,v_j|G^t)+\sum_{i=1}^{n_1}\sum_{j=1}^{n_1}d(v_i,v_j|G^t)\right\}$$
$$=\frac{1}{2}\left\{2IW(G)+2n_1(n_1-1)+2\sum_{i=1}^{n_1'}\sum_{j=1}^{n_0}d(v_i,v_j)\right.$$
$$+2TW(G)\}$$
$$=\{2IW(G)+2n_1(n_1-1)$$
$$+[2W(G)-2WI(G)-2TW(G)+2n_1n_0]+2TW(G)\}$$
$$\{2W(G)+2n_1(n_1-1)+2n_1n_0\}$$
$$TW(G^t)=W(G)+n_1(n_1+n_0-1).$$

■

III. Observation and Analysis

Caterpillar graph is a tree in which all the vertices of the caterpillar are within distance one from the main path. In the main path the vertex set be $v_1,v_2,\ldots,v_n$. Caterpillar tree is isomorphic to certain types of molecular graphs. Consider a saturated hydrocarbon with n carbon atoms there are k methyl molecules attached in various positions i, $(2\leq i\leq n-1)$.

Theorem 10: If T be a caterpillar with n vertices on the main path having k pendent edges at various positions i $(2\leq i\leq n-1)$, then $TW(G)=(k+1)(n+k-1)+\dfrac{1}{2}\sum_{i}\sum_{i_k}|i_i-i_k|$.

Proof: Let $T(n,k)$ be a caterpillar graph with $n+k$ vertices, $\{v_1,v_2,\ldots,v_n\}$ be the vertices on the main path. The degree sequence of a caterpillar graph is $(d_1,d_2,\ldots,d_n,d_{n+1},d_{n+2},\ldots,d_{n+k})$. The degree sequence on the main path $\{d_i\}_{i=2}^{n-1}$ is either 2 or 3. The degree sequence of $d_1,d_n,d_{n+1},d_{n+2},\ldots,d_{n+k}$ is one. The positions of k pendent edges lies on the main path in various position is v_2 to v_{n-1}. The Terminal Wiener index of a graph is sum of the distance between v_1^{th} and v_n^{th} vertex, sum of the distance between pairs of k pendent vertices and sum of the distance between v_1 and v_n^{th} vertex to k pendent vertices.

$$TW(T)=\frac{1}{2}\left\{2(n-1)+\sum_{i_1}\sum_{i_k}|i_i-i_k|+2k(k-1)\right.$$
$$\left.+2\sum_{i_1}|1-i_1|+2\sum_{i_1}|n-i_1|+2(2k)\right\}$$
$$TW(T)=\frac{1}{2}\left\{2(n-1)+2k(k+1)+\sum_{i_1}\sum_{i_k}|i_1-i_k|\right.$$
$$\left.-2\sum_{i_1}|1-i_1|+2\sum_{i_1}|n-i_1|\right\}$$
$$TW(T)=(n-1)+k(k+1)+\frac{1}{2}\sum_{i_1}\sum_{i_k}|i_i-i_k|+(nk-k)$$
$$TW(T)=(k+1)(n+k-1)+\frac{1}{2}\sum_{i_1}\sum_{i_k}|i_i-i_k|.$$

■

Example 1:

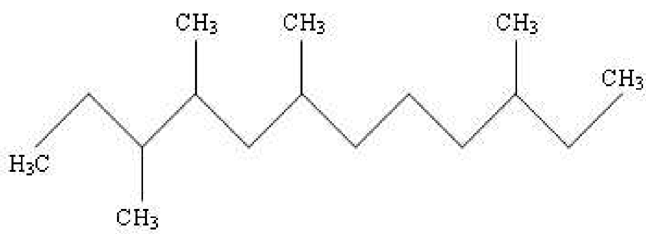

Fig. 1. (3, 4, 6, 10) - tetramethyldodecane

If we can study that for all molecules, the distance between two extremum methyl molecules as well as the two intermediate methyl molecules have the same distance contain same Terminal Wiener index.

If we denote (a,b,c,d)-tetramethyldodecane in the following table, where (a,b,c,d) denote the positions of the 4 methyl molecules varying over the positions from 2 to n-1 in the straight chain consisting of n carbon atoms. In the molecular structure 3, 4, 6, 10 tetramethyldodecane, the distance between the positions of (3, 10) and (4, 6) are 7 and 2 respectively. The positions of the molecular structure (2, 3, 5, 9) and (4, 5, 7, 11) of tetramethyldodecane, the Terminal Wiener Index is similar.

TABLE I
TERMINAL WIENER INDEX FOR CERTAIN CHEMICAL COMPOUNDS

S.No.	Chemical compound tetramethyldodecane	TW(G)
1	(2,3,4,7), (3,4,5,8), (3,6,7,8), (4,7,8,9), (5,8,9,10), (6,9,10,11)	91
2	(2,4,6,7), (3,5,7,8), (4,6,8,9), (5,7,9,10), (6,8,10,11), (2,3,5,7), (3,4,6,8), (4,5,7,9), (5,6,8,10), (6,7,9,11)	92
3	(2,3,6,7), (3,4,7,8), (4,5,8,9), (5,6,9,10), (6,7,10,11)	93
4	(2,3,4,8), (3,4,5,9), (4,5,6,10), (5,6,7,11), (2,6,7,8), (3,7,8,9), (4,8,9,10), (5,9,10,11), (2,4,5,8), (3,5,6,9), (4,6,7,10), (5,7,8,11), (2,5,6,8), (3,6,7,9), (4,7,8,10), (5,8,9,11)	94
5	(2,4,6,8), (3,5,7,9), (4,6,8,10), (5,7,9,11), (2,3,5,8), (3,4,6,9), (4,5,7,10), (5,6,8,11), (2,5,7,8), (3,6,8,9) (5,8,10,11), (4,7,9,10)	95
6	(2,3,6,8), (3,4,7,9), (4,5,8,10), (5,6,9,11), (2,4,7,8), (3,5,8,9), (4,6,9,10), (5,7,10,11)	96
7	(2,3,4,9), (3,4,5,10), (4,5,6,11), (2,4,5,9), (3,5,6,10), (4,6,7,11), (2,5,6,9), (3,6,7,10), (4,7,8,11), (2,6,7,9), (3,7,8,10), (4,8,9,1), (2,7,8,9), (3,8,9,10)	97
8	(2,3,5,9), (3,4,6,10), (4,5,7,11), (2,4,6,9), (3,5,7,10), (4,6,8,11), (2,5,7,9), (3,6,8,10), (4,7,9,11), (2,6,8,9) (3,7,9,10), (4,8,10,11)	98
9	(2,3,6,9), (3,4,7,10), (4,5,8,11), (2,4,7,9), (3,5,8,10), (4,6,9,11), (2,5,8,9), (2,6,9,10), (4,7,10,11)	99
10	(2,3,4,10), (3,4,5,11), (2,4,8,9), (3,5,9,10), (4,6,10,11), (2,3,7,9), (3,4,8,10), (4,5,9,11)	100

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J. Baskar Babujee received M.Sc., M.Phil., from Madras Christian College, Chennai in 1991 and 1992 respectively. He received his Ph.D., degree in 2004 from Jawaharlal Nehru Technological University, Hyderabad, India. He has 160 publications in academic journals and international conference proceedings. He is currently an Associate Professor in the Department of Mathematics, Anna University, Chennai, India. His current research interest includes Graph theory, Cryptography, Formal languages and Automata theory.

J. Senbagamalar received her M.Sc degree (2002) M.Phil degree (2003) in Mathematics from Madurai Kamaraj University, Madurai, India in 2003. Currently she is working towards her Ph.D. degree in the area of Topological indices on Chemical Graph Theory at Department of Mathematics, Anna University, India.