*MATCH*
*Communications in Mathematical and in Computer Chemistry*

MATCH Commun. Math. Comput. Chem. **67** (2012) 331-336

ISSN 0340 - 6253

# On the Wiener Index and Circumference*

**Xiaoxia Lin** †

*School of Sciences, Jimei University, Xiamen, Fujian, 361021, P. R.China*

(Received March 28, 2011)

**Abstract**

The Wiener index of a graph is defined as the sum of distances between all pairs of vertices of the graph. In this paper, we bound the Wiener index in a connected graph in function of its order and circumference, the graphs which minimize and maximize the Wiener index among all graphs with given order and circumference are also characterized.

## 1 Introduction

All graphs considered in this paper are simple, connected graphs. Let $G$ be a graph and $e(G)$ the number of edges of $G$. The circumference of $G$, $c(G)$, is the maximum length of a cycle in $G$. A block of $G$ is either a maximal 2-connected subgraph of $G$ or a cut edge of $G$. Denote by $G(n, l)$ the set of graphs with $n$ vertices and circumference $l$. The diameter of $G$ is the maximum distance between two vertices of $G$. The distance of a vertex $v$, $d_G(v)$, is the sum of distances between $v$ and all other vertices of $G$. The number of vertex pairs at distance $k$ in $G$ is denoted by $d(G, k)$. A vertex of degree one will be called a pendent vertex. Let $K_n$ and $P_n$ denote the complete graph and path on $n$ vertices, respectively. We refer the readers to [4] for other terminologies and notations not defined here.

The Wiener index, $W(G)$, is the sum of distances between all pairs of vertices of a graph $G$. It is one of the oldest topological indices which was first introduced by Wiener [16] and has been extensively studied in the literature since the middle of the 1970s.

*This project is supported by the Natural Science Foundation of Fujian Province of China (No. 2010J01008) and NSFC (11001113)

†E–mail: lxx@jmu.edu.cn

Numerous of its chemical applications and mathematical properties are well studied [1, 6-8, 13-15]. For detailed results on this topic, the readers could be referred to [6, 7]. A closed concept related to Wiener index is the mean distance. For an $n-$ vertex graph $G$, the mean distance is defined as $\mu(G) = W(G)/\binom{n}{2}$. Mean distance is used in studying efficiency of networks, good networks are often characterized by a small distance.

In the investigation of Wiener index of graphs, many interesting extremal results have been found. Entringer et. al [8] proved that if $T_n$ is a tree on $n$ vertices, then $(n-1)^2 \leq W(T_n) \leq \binom{n+1}{3}$, and the upper bound is achieved if and only if $T_n \cong P_n$ and the lower bound is achieved if and only if $T_n \cong K_{1,n-1}$. J. Plesník [13] determined the lower bound of Wiener index in the class of graphs with $n$ vertices and diameter $d$, and proved that among all 2-connected graphs of a given order $n$ the Wiener index is maximized by the cycle $C_n$. H. B. Walikar, V. S. Shigehall, H. S. Ramane [15] gave some upper and lower bounds on the Wiener index of a graph in terms of some graph-theoretic parameters, like radius, diameter, order, size, independence number, connectivity and chromatic number. On the other hands, some extremal results on mean distance are also established. In [5], Chung has showed that the mean distance is at most as large as the independence number, which was a conjecture of the widely known Graffiti program of Fajtlowicz [10]. Kouider and Winkler have used the minimum degree to bound the upper bound of mean distance [12]. Recently, Bekkai and Kouider gave the lower and upper bounds on the mean distance in a connected graph in terms of its order and girth [2].

In this paper, we give the upper and lower bounds on the Wiener index of a graph in term of its order and circumference. The extremal graphs which minimize and maximize the Wiener index among all graphs with given order and circumference are also characterized.

# 2 Lemmas and results

We first introduce some classes of graphs and lemmas which will help to prove our main result. Given two numbers $a$ and $b$, if $a$ divides $b$, we use the notation $a|b$.

Let $n$ and $l$ be two positive integers such that $(l-1)|(n-1)$. We use $S(n,l)$ to denote the following class of graphs: each of which has $\frac{n-1}{l-1}$ blocks and every block is a complete graph $K_l$. $S^*_{n,l}$ denotes the following graph: take $\frac{n-1}{l-1}$ disjoint copies of the complete graph $K_{l-1}$, add a vertex $u$ and join $u$ to every vertex of those complete graphs.

It is easily checked that $S(n,l) \subseteq G(n,l)$ and $S^*_{n,l}$ is the unique graph in $S(n,l)$ with diameter 2. Some of these graphs are depicted in Fig.1.

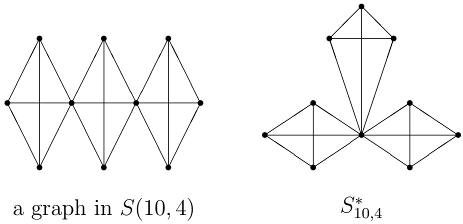


**Fig. 1 Some graphs of** $S(10,4)$

Let $C_r \cdot P_t$ be the graph obtained from a $r-$ vertex cycle $C_r$ and $P_t$ by joining a vertex of $C_r$ to one end vertex of $P_t$. In Fig.2, we have drawn $C_3 \cdot P_4$.

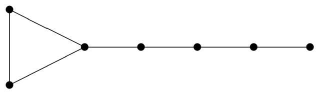

**Fig. 2** $C_3 \cdot P_4$

The following well-known theorem proved by Erdős and Gallai in 1959 is a classical result in extremal graph theory, see [3, Chapter 3] or see [9] for details.

**Lemma 1 ([3, 9]).** Let $G$ be a graph on $n$ vertices with $c(G) \le l$. Then

$$e(G) \le (n-1)l/2$$

and the equality holds if and only if $(l-1)|(n-1)$ and $G \in S(n,l)$ .

**Lemma 2 ([14]).** $W(C_{2n}) = \dfrac{(2n)^3}{8}$ , $W(C_{2n+1}) = \dfrac{(2n+2)(2n+1)(2n)}{8}$ .

**Lemma 3 ([6]).** $W(P_n) = \binom{n+1}{3}$ .

**Lemma 4 ([1]).** Let $G$ be a connected graph with a cut-vertex $u$ such that $G_1$ and $G_2$ are two connected subgraphs of $G$ having $u$ as the only common vertex and $G_1 \cup G_2 = G$. Let $n_1 = |V(G_1)|$ and $n_2 = |V(G_2)|$. Then

$$W(G) = W(G_1) + W(G_2) + (n_1 - 1)\, d_{G_2}(u) + (n_2 - 1)\, d_{G_1}(u) \ .$$

**Lemma 5.** Let $n$ and $l$ be two positive integers such $n > l$. Then

$$W(C_l \cdot P_{n-l}) = k^3 + \binom{n-2k+2}{3} + \frac{(n-2k)(n-2k+1)(2k-1)}{2} + (n-2k)k^2$$

if $l = 2k,\ k = 2, 3, \ldots,$ and

$$W(C_l \cdot P_{n-l}) = \frac{(k+1)(2k+1)k}{2} + \binom{n-2k+1}{3} + (n-2k-1)(nk-k^2+k)$$

if $l = 2k+1,\ k = 1, 2, \ldots.$

**Proof.** Suppose $u$ is the unique vertex in $C_l \cdot P_{n-l}$ with degree 3. Set $G_1 = C_l$ and $G_2 = P_{n-l-1}$. Thus $G_1$ and $G_2$ are two connected subgraphs of $C_l \cdot P_{n-l}$ having $u$ as the only common vertex and $G_1 \cup G_2 = C_l \cdot P_{n-l}$. Applying Lemma 2, Lemma 3 and Lemma 4 can give the result. □

Now we are in the position to state the main result of this paper.

When $n = l$, among all graphs in $G(n, l)$, it is easily seen that the Wiener index is maximized by the cycle $C_n$ and minimized by the complete graph $K_n$. So in the following, we only consider the graph $G$ with $n$ vertices and $c(G) = l \leq n-1$. Define

$$f(n,l) = k^3 + \binom{n-2k+2}{3} + \frac{(n-2k)(n-2k+1)(2k-1)}{2} + (n-2k)k^2$$

if $l = 2k,\ k = 2, 3, \ldots,$ and

$$f(n,l) = \frac{(k+1)(2k+1)k}{2} + \binom{n-2k+1}{3} + (n-2k-1)(nk-k^2+k)$$

if $l = 2k+1,\ k = 1, 2, \ldots.$

Then we have the following result.

**Theorem 6.** Let $G \in G(n, l)$, where $n > l$. Then

$$n(n-1) - \frac{(n-1)l}{2} \leq W(G) \leq f(n,l)\ .$$

The lower bound is achieved if and only if $(l-1)|(n-1)$ and $G \cong S^*_{n,l}$, the upper bound is achieved if and only if $G \cong C_l \cdot P_{n-l}$.

**Proof.** Suppose the diameter of $G$ is $d$. Then the Wiener index of $G$ can be expressed as:

$$W(G) = \sum_{i=1}^{d} i\, d(G,i)\ .$$

The number of vertex pairs at unit distance in $G$ is equal to the number of edges of $G$. Thus, $d(G,1) = e(G)$ . Therefore,

$$W(G) \;=\; d(G,1) + \sum_{i=2}^{d} i\, d(G,i) = e(G) + \sum_{i=2}^{d} i\, d(G,i) \geq e(G) + 2\sum_{i=2}^{d} d(G,i) \quad (1)$$

$$
\begin{aligned}
&= e(G) + 2\left[\sum_{i=1}^{d} d(G,i) - d(G,1)\right] = e(G) + 2\left[\binom{n}{2} - e(G)\right] \\
&= n(n-1) - e(G) \geq n(n-1) - \frac{(n-1)l}{2} \qquad \text{(by Lemma 1)} \; . \qquad (2)
\end{aligned}
$$

It is evident that the equality in (1) will hold if and only if the diameter of $G$ is 2. By Lemma 1, the equality in (2) will hold if and only if $(l-1)|(n-1)$ and $G \in S(n,l)$. Note that $S^*_{n,l}$ is the unique graph in $S(n,l)$ with diameter 2. So

$$W(G) \geq n(n-1) - \frac{(n-1)l}{2} \, ,$$

and the discussion above implies that the equality holds if and only if $(l-1)|(n-1)$ and $G \cong S^*_{n,l}$.

In the following, we will prove the upper bound on $W(G)$ by induction on $n$.

Let $G^*$ be a graph with maximum Wiener index in the class $G(n,l)$ and $C$ a cycle of length $l$ in $G^*$. Since $n > l$, and $G^*$ maximizes the Wiener index, it is easy to see that there exists a vertex $u \in V(G^*) \setminus V(C)$ such that $u$ a pendent vertex of $G^*$.

Because the vertex pairs of $G^*$ can be divided into two groups: those which do not contain $u$ and those which do contain $u$. The sum of distances of the vertex pairs of the first type is just the Wiener index of the graph $G^* - u$. So

$$W(G^*) = W(G^* - u) + d_{G^*}(u) \; .$$

Let $v$ be the pendent vertex of $C_l \cdot P_{n-l}$. Similarly, we have

$$W(C_l \cdot P_{n-l}) = W(C_l \cdot P_{n-l} - v) + d_{C_l \cdot P_{n-l}}(v) = W(C_l \cdot P_{n-l-1}) + d_{C_l \cdot P_{n-l}}(v) \; .$$

Clearly, $G^* - u \in G(n-1,l)$, by the induction hypothesis, $W(G^* - u) \leq W(C_l \cdot P_{n-l-1})$. It is easily checked that $d_{G^*}(u) \leq d_{C_l \cdot P_{n-l}}(v)$ with the equality holding if and only if $G^* \cong C_l \cdot P_{n-l}$. So, $W(G^*) \leq W(C_l \cdot P_{n-l})$, and the equality holds if and only if $G^* \cong C_l \cdot P_{n-l}$. By Lemma 5, $W(C_l \cdot P_{n-l}) = f(n,l)$. Therefore,

$$W(G) \leq f(n,l)$$

and the equality holds if and only if $G \cong C_l \cdot P_{n-l}$. ■

## References

[1] R. Balakrishnan, N. Sridharan, K. V. Iyer, Wiener index of graphs with more than one cut-vertex, *Appl. Math. Lett.* **21** (2008) 922–927.

[2] S. Bekkai, M. Kouider, On mean distance and girth, *Discr. Appl. Math.* **158** (2010) 1888–1893.

[3] B. Bollobás, *Extremal Graph Theory*, Academic Press, New York, 1978.

[4] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Macmillan, London, 1976.

[5] F. R. K. Chung, The average distance and the independence number, *J. Graph Theory* **12** (1988) 229–235.

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

[7] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.

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

[9] P. Erdős, T. Gallai, On maximal paths and circuits of graphs, *Acta Math. Acad. Sci. Hungar.* **10** (1959) 337–356.

[10] S. Fajtlowicz, Written on the wall, Department of Mathematics, University of Houston, http://math.uh.edu/∼clarson/graffiti.html.

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

[12] M. Kouider, P. Winkler, Mean distance and minimum degree, *J. Graph Theory* **25** (1999) 95–99.

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

[14] B. E. Sagan, Y. N. Yeh, P. Zhang, The Wiener polynomial of a graph, *Int. J. Quant. Chem.* **60** (1996) 959–969.

[15] H. B. Walikar, V. S. Shigehalli, H. S. Ramane, Bounds on the Wiener number of a graph, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 117–132.

[16] H. Wiener, Structual determination of paraffin boiling points, *J. Amer. Chem. Soc.* **69** (1947) 17–20.