Discrete Mathematics Letters
www.dmlett.com

Discrete Math. Lett. **9** (2022) 44–48
DOI: 10.47443/dml.2021.s208

Research Article

On the Wiener index of two families generated by joining a graph to a tree

Andrey A. Dobrynin*

Sobolev Institute of Mathematics, Siberian Branch of the Russian Academy of Sciences, Novosibirsk, 630090, Russia

(Received: 17 January 2022. Accepted: 26 January 2022. Published online: 2 February 2022.)

Abstract

The Wiener index $W(G)$ of a graph G is the sum of distances between all vertices of G. The Wiener index of a family of connected graphs is defined as the sum of the Wiener indices of its members. Two families of graphs can be constructed by identifying a fixed vertex of an arbitrary graph F with vertices or subdivision vertices of an arbitrary tree T of order n. Let G_v be a graph obtained by identifying a fixed vertex of F with a vertex v of T. The first family $\mathcal{V} = \{G_v \,|\, v \in V(T)\}$ contains n graphs. Denote by G_{v_e} a graph obtained by identifying the same fixed vertex of F with the subdivision vertex v_e of an edge e in T. The second family $\mathcal{E} = \{G_{v_e} \,|\, e \in E(T)\}$ contains $n-1$ graphs. It is proved that $W(\mathcal{V}) = W(\mathcal{E})$ if and only if $W(F) = 2W(T)$.

Keywords: graph invariant; distance in graphs; Wiener index.

2020 Mathematics Subject Classification: 05C09, 05C12, 05C92.

1. Introduction

In this paper we are concerned with undirected connected graphs G with vertex set $V(G)$ and edge set $E(G)$. The *order* n_G of a graph G is the number of its vertices. By *distance* $d_G(u,v)$ between vertices u and v of G we mean the number of edges in a shortest path connecting them. Denote by $d_G(v)$ the sum of distances from a vertex v to all vertices of G. The *Wiener index* is a topological index based on distances between vertices of a graph G:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v) = \frac{1}{2} \sum_{v \in V(G)} d_G(v).$$

It was introduced to quantify the structural information of tree-like molecular graphs [25] and have found numerous applications in organic chemistry and other fields. In particular, the Wiener index was used for the design of quantitative structure-property relations for chemical compounds [1,2,17,20,21]. The success in the application of this index has been the reason for the intensive study of its mathematical properties. The comprehensive bibliography regarding this index can be found in books [3,14,22–24] and reviews [2,9,11–13,15,16,18].

In this paper, we study the Wiener index for two families of graphs. These families arise as a result of structural transformations of a graph. The Wiener index of a family $\mathcal{G}$ of connected graphs $\mathcal{G} = \{G_1, G_2, \ldots, G_k\}$ is defined as the sum of the Wiener indices of its members,

$$W(\mathcal{G}) = W(G_1) + W(G_2) + \cdots + W(G_k).$$

The *subdivision of an edge* e in a tree T is the replacement of e with a new path of order 3. The resulting tree T_e contains one more edge than T. The central vertex v_e of the path is called the *subdivision vertex*. Denote by P_n, C_n, S_n, and $S_{a,b,c}$ the path, the cycle, the star of order n and the generalized star with branches of length a, b, c and order $n = a+b+c+1$.

Two families of graphs can be constructed by identifying a fixed vertex of an arbitrary graph F with vertices or subdivision vertices in an arbitrary tree T. Let G_v be a graph obtained by identifying a fixed vertex u of F with a vertex v of T. The first family $\mathcal{V} = \{G_v \,|\, v \in V(T)\}$ contains n graphs of order $n_T + n_F - 1$ (see the left part of Figure 1). Denote by G_{v_e} a graph obtained by identifying the same fixed vertex u of F with the subdivision vertex v_e of an edge e in T. The second family $\mathcal{E} = \{G_{v_e} \,|\, e \in E(T)\}$ contains $n-1$ graphs with $n_T + n_F$ vertices (see the right part of Figure 1). We are interesting in finding conditions for the coincidence the Wiener indices of families $\mathcal{V}$ and $\mathcal{E}$.

*E-mail address: dobr@math.nsc.ru

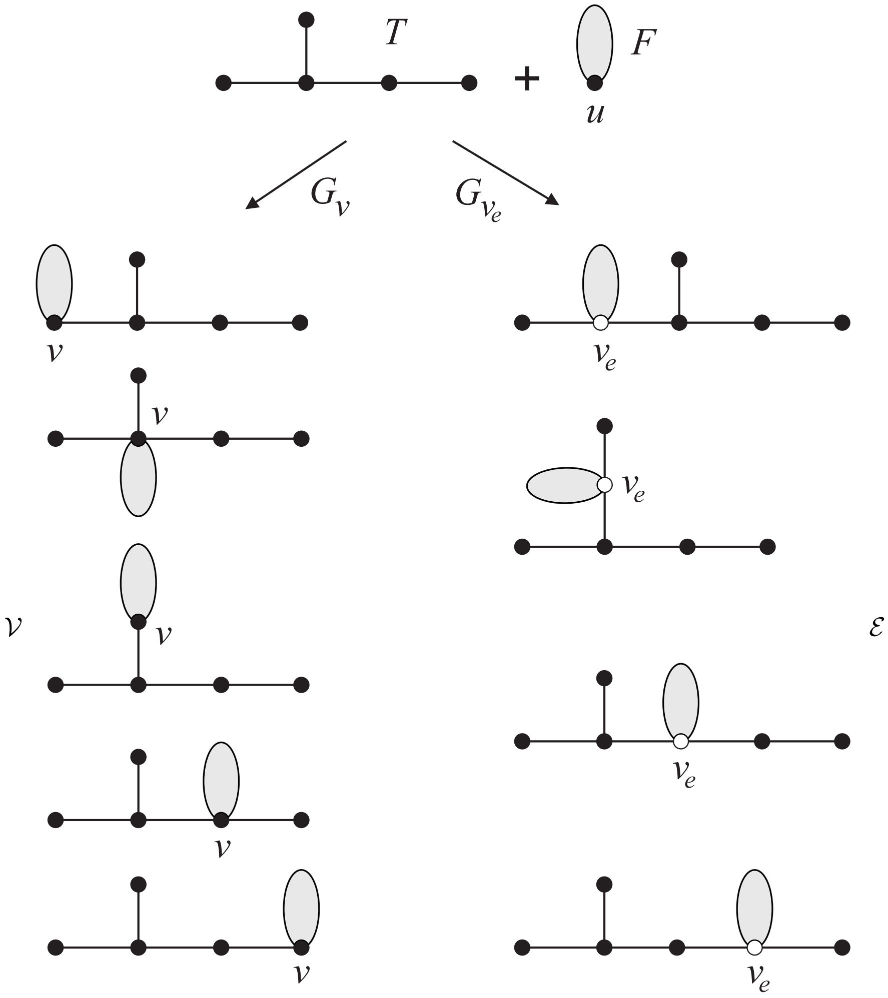

Figure 1: Families $\mathcal{V}$ and $\mathcal{E}$ of graphs obtained by joining a tree T and a graph F.

2. Main result

We need two useful results concerning Wiener index of the family of trees obtained from a tree by subdivisions of its edges. Subdivisions of edges of a tree T form a family containing trees $T_e, e \in E(T)$. The following result was proved in [7]:

Lemma 2.1. *For the family $T_{e_1}, T_{e_2}, \dots, T_{e_{n-1}}$ of all edge subdivisions of a tree T of order n,*

$$W(T_{e_1}) + W(T_{e_2}) + \cdots + W(T_{e_{n-1}}) = (n+2)W(T).$$

It is known that the sum of the distances of all subdivision vertices v_e of edges $e \in E(T)$ is twice the Wiener index [7].

Lemma 2.2. *For the subdivision vertices $v_{e_1}, v_{e_2}, \dots, v_{e_{n-1}}$ of edges in a tree T of order n,*

$$d_{T_{e_1}}(v_{e_1}) + d_{T_{e_2}}(v_{e_2}) + \cdots + d_{T_{e_{n-1}}}(v_{e_{n-1}}) = 2W(T).$$

Let families $\mathcal{V} = \{G_v \,|\, v \in V(T)\}$ and $\mathcal{E} = \{G_{v_e} \,|\, e \in E(T)\}$ are obtained from an arbitrary tree T and a graph F as described above (see Figure 1).

Theorem 2.1. *The Wiener indices of the families $\mathcal{V}$ and $\mathcal{E}$ coincide, $W(\mathcal{V}) = W(\mathcal{E})$, if and only if $W(F) = 2W(T)$.*

Proof. Let graph G_v be obtained by identifying a vertex $v \in V(T)$ and a vertex $u \in V(F)$. Then $W(G_v)$ can be presented as follows [19]

$$W(G_v) = W(T) + W(F) + (n_T - 1)d_F(u) + (n_F - 1)d_T(v).$$

Summing this equation for all vertices $v \in V(T)$, we have

$$\begin{aligned} W(\mathcal{V}) = \sum_{v \in V(T)} W(G_v) &= n_T W(T) + n_T W(F) + n_T(n_T - 1)d_F(u) + (n_F - 1) \sum_{v \in V(T)} d_T(v) \\ &= n_T W(T) + n_T W(F) + n_T(n_T - 1)d_F(u) + 2(n_F - 1)W(T) \end{aligned}$$

$$= (n_T + 2n_F - 2)W(T) + n_T W(F) + n_T(n_T - 1)d_F(u).$$

Let graph G_e be obtained by identifying the subdivision vertex v_e of T_e and a vertex $u \in V(F)$. Then

$$\begin{aligned} W(G_e) &= W(T_e) + W(F) + (n_{T_e} - 1)d_F(u) + (n_F - 1)d_{T_e}(v_e) \\ &= W(T_e) + W(F) + n_T d_F(u) + (n_F - 1)d_{T_e}(v_e). \end{aligned}$$

Summing this equation for all edges $v \in E(T)$, we get

$$W(\mathcal{E}) = \sum_{e \in E(T)} W(G_e) = \sum_{e \in E(T)} W(T_e) + (n_T - 1)W(F) + n_T(n_T - 1)d_F(u) + (n_F - 1) \sum_{e \in E(T)} d_{T_e}(v_e).$$

Applying Lemmas 2.1 and 2.2, we can write

$$\begin{aligned} W(\mathcal{E}) &= (n_T + 2)W(T) + (n_T - 1)W(F) + n_T(n_T - 1)d_F(u) + 2(n_F - 1)W(T) \\ &= (n_T + 2n_F)W(T) + (n_T - 1)W(F) + n_T(n_T - 1)d_F(u). \end{aligned}$$

Therefore, $W(\mathcal{V}) - W(\mathcal{E}) = W(F) - 2W(T)$. □

As an illustration, consider two families of unicyclic graphs obtained from a tree T and a graph F for which $W(F) = 2W(T) = 64$ (see Figures 2 and 3). Wiener indices are indicated near graph diagrams. By Theorem 2.1, these families must have the same Wiener index. Indeed, $W(\mathcal{V}) = 290+262+290+262+276+304 = 1684$ and $W(\mathcal{E}) = 337+337+325+332+353 = 1684$.

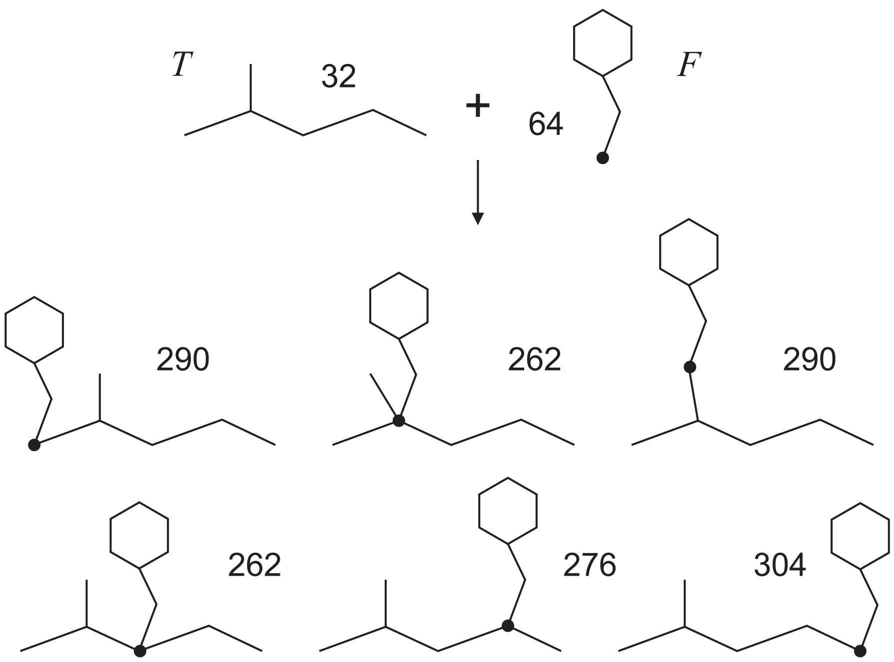

Figure 2: Family $\mathcal{V}$ of unicyclic graphs with $W(\mathcal{V}) = 1684$.

If T and F are both trees and $W(F) = 2W(T)$, then their minimal order are 4 and 5, respectively. Namely, $W(T) = W(P_4) = 10$ and $W(F) = W(P_5) = 20$ or $W(T) = W(S_4) = 10$ and $W(F) = W(S_{1,1,2}) = 20$. If such trees have the same order, then the smallest trees are the star S_{11} and the generalized star $S_{1,4,5}$ for which $W(T) = W(S_{11}) = 100$ and $W(F) = W(S_{1,4,5}) = 200$.

The above considerations may be useful for estimating how the Wiener index changes on average under attaching a graph F to a tree T. The resulting expressions do not depend on local distance characteristics of tree vertices:

$$W_{\mathrm{avr}}(\mathcal{V}) = \frac{W(\mathcal{V})}{n_T} = \left(1 + \frac{2n_F - 2}{n_T}\right) W(T) + W(F) + (n_T - 1)d_F(u),$$

$$W_{\mathrm{avr}}(\mathcal{E}) = \frac{W(\mathcal{E})}{n_T - 1} = \left(1 + \frac{2n_F + 1}{n_T - 1}\right) W(T) + W(F) + n_T d_F(u).$$

For the smallest graph $F \cong P_2$,

$$W_{\mathrm{avr}}(\mathcal{V}) = \left(1 + \frac{2}{n_T}\right) W(T) + n_T$$

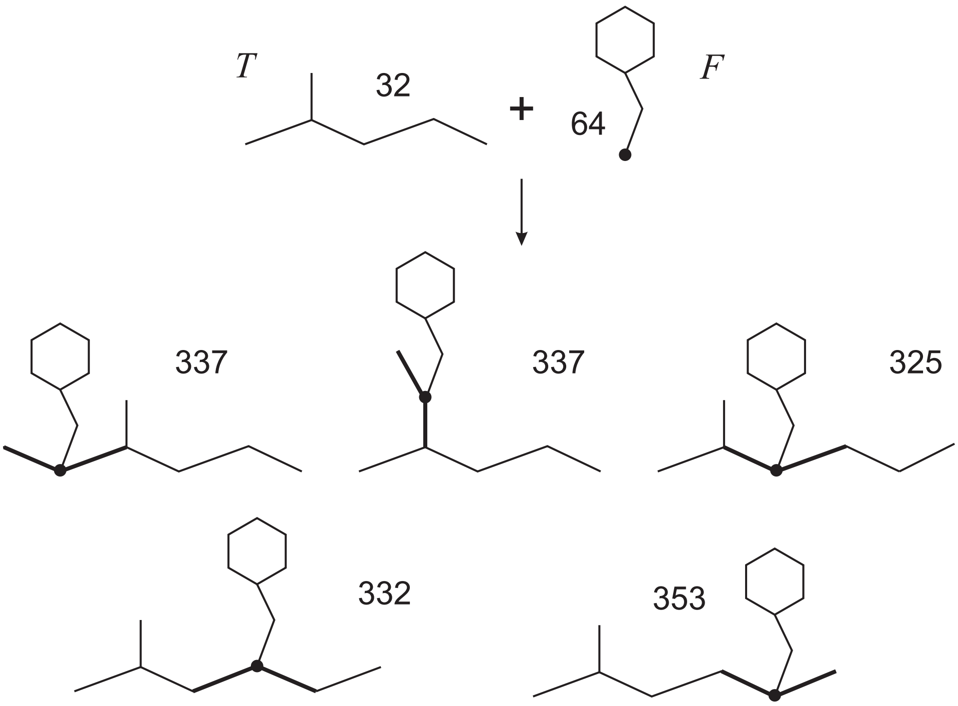

Figure 3: Family $\mathcal{E}$ of unicyclic graphs with $W(\mathcal{E}) = 1684$.

and

$$W_{\rm avr}(\mathcal{E}) = \left(1 + \frac{5}{n_T - 1}\right) W(T) + n_T + 1.$$

Values $W_{\rm avr}(\mathcal{V})$ or $W_{\rm avr}(\mathcal{E})$ may be integer. Coefficients at $W(T)$ are equal to 2 if $n_F = n_T/2 + 1$ or $n_F = n_T/2 - 1$ for even n_T. Since $W(P_n) = n(n-1)(n+1)/6$, both quantities $W_{\rm avr}(\mathcal{V})$ and $W_{\rm avr}(\mathcal{E})$ are integers if $T \cong P_{6m-1}$, $m \geq 1$. Average values of the Wiener index may be realized by graphs. Let families $\mathcal{V}$ and $\mathcal{E}$ be constructed using $T \cong P_7$, $F \cong P_2$ and $T \cong P_9$, $F \cong C_6$, respectively. Then $W_{\rm avr}(\mathcal{V}) = 79$ and $W_{\rm avr}(\mathcal{E}) = 339$ are realized by graphs of $\mathcal{V}$ and $\mathcal{E}$.

3. Conclusion

In the presented paper, we have studied properties of the Wiener index for two families of graphs. Properties of this kind can be regarded as collective properties of the Wiener index, i.e. the main results don't reflect the property of the index of any particular graph, but a collective property of families of such graphs. This approach may be useful in studying of topological indices of mixtures of molecular graphs or in characterizing sets of graphs obtained after destruction of complex formations. Some results in this direction have been reported for trees and hexagonal chains in [4–8, 10].

Acknowledgment

This study was carried out within the framework of the state contract of the Sobolev Institute of Mathematics (project number FWNF-2022-0017).

References

[1] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topological indices for structure-activity correlations, *Topics Curr. Chem.* **114** (1983) 21–55.
[2] D. Bonchev, The Wiener number – Some applications and new developments, In: D. H. Rouvray, R. B. King (Eds.), *Topology in Chemistry: Discrete Mathematics of Molecules*, Horwood, Chichester, 2002, pp. 58–88.
[3] D. Bonchev, D. H. Rouvray (Eds.), *Chemical Graph Theory: Introduction and Fundamentals*, Gordon & Breach, New York, 1991.
[4] A. A. Dobrynin, On the Wiener index of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 707–726.
[5] A. A. Dobrynin, On the Wiener index of certain families of fibonacenes, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 565–574.
[6] A. A. Dobrynin, Wiener index of hexagonal chains with segments of equal length, In: M. Dehmer, F. Emmert-Streib (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications*, Chapman & Hall/CRC, New York, 2014, pp. 81–109.
[7] A. A. Dobrynin, Wiener index of subdivisions of a tree, *Sib. Èlektron. Mat. Izv.* **16** (2019) 1581–1586.
[8] A. A. Dobrynin, On the Wiener index of the forest induced by contraction of edges in a tree, *MATCH Commun. Math. Comput. Chem.* **86** (2020) 321–326.
[9] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.
[10] A. A. Dobrynin, E. Estaji, Wiener index of certain families of hexagonal chains, *J. Appl. Math. Comput.* **59** (2019) 245–256.
[11] A. A. Dobrynin, I. Gutman, S. Klavžar, P. Žigert, Wiener index of hexagonal systems, *Acta Appl. Math.* **72** (2002) 247–294.
[12] A. A. Dobrynin, L. S. Mel'nikov, Wiener index of line graphs, In: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs – Theory*, Univ. Kragujevac, Kragujevac, 2012, pp. 85–121.

[13] R. C. Entringer, Distance in graphs: Trees, *J. Combin. Math. Combin. Comput.* **24** (1997) 65–84.
[14] I. Gutman, O. E. Polansky, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1986.
[15] M. Knor, R. Škrekovski, Wiener index of line graphs, In: M. Dehmer, F. Emmert-Streib (Eds.), *Quantitative Graph Theory: Mathematical Foundations and Applications*, Chapman & Hall/CRC, New York, 2014, pp. 279–301.
[16] M. Knor, R. Škrekovski, A. Tepeh, Mathematical aspects of Wiener index, *Ars Math. Contemp.* **11** (2016) 327–352.
[17] B. Lučić, I. Lukovits, S. Nikolić, N. Trinajstić, Distance-related indexes in the quantitative structure-property relationship, *J. Chem. Inf. Comput. Sci.* **41** (2001) 527–535.
[18] S. Nikolić, N. Trinajstić, Z. Mihalić, The Wiener index: Developments and applications, *Croat. Chem. Acta* **68** (1995) 105–129.
[19] O. E. Polansky, D. Bonchev, The Wiener number of graphs. I. General theory and changes due to some graph operations, *MATCH Commun. Math. Comput. Chem.* **21** (1986) 133–186.
[20] D. H. Rouvray, Should we have designs on topological indices?, In: R. B. King (Ed.), *Chemical Application of Topology and Graph Theory*, Elsevier, Amsterdam, 1983, pp. 159–177.
[21] D. H. Rouvray, The modelling of chemical phenomena using topological indices, *J. Comput. Chem.* **8** (1987) 470–480.
[22] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.
[23] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1982 (Second Edition, 1992).
[24] S. Wagner, H. Wang, *Introduction to Chemical Graph Theory*, Chapman & Hall/CRC, Boca Raton, 2018.
[25] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.