



An Efficient Computational Method for a Distance-based Measure of Graphenylene Networks

Meryam Zeryouh¹, Mohamed El Marraki¹, Mohamed Essalih^{1,2}

¹LRIT - CNRST URAC 29, Rabat IT Center - Faculty of sciences, MOHAMMED V UNIVERSITY IN RABAT, B.P 1014, Rabat, Morocco.

²LAPSSII, The Safi's Graduate School of Technology, CADI AYYAD UNIVERSITY IN MARRAKESH, Marrakesh, Morocco.

zeryouh.meryam@gmail.com

marraki@fsr.ac.ma

essalih.mohamed@yahoo.fr

ABSTRACT

Topological indices are considered as effective measures for analyzing and quantifying the topological structure of networks. Recently, many methods were proposed for calculating distance-based topological indices. In this article, the computation efficiency of a measure named the generalized Terminal Wiener index is investigated. At first, we present a method that calculates the generalized Terminal Wiener index of a specific class of graphs and particularly the graphenylene systems in a linear time complexity. After that, we use the proposed technique to analyze the structural properties of two graphenylene networks, called the graphenylene chain network GC_n and the graphenylene sheet network GS_n .

Key words: Topological indices, Network, Generalized Terminal Wiener, Graphenylene, Computational complexity.

1. INTRODUCTION

Nowadays, the topological indices are investigated as a fundamental tool to characterize and represent the structural properties of any network in quantitative terms [1]. For instance, they have been used to analyze the chemical structure of molecules, the social networks, the interconnection networks and many other networks from different fields. The theory of topological indices began in 1947, when the physical chemist H. Wiener used the Wiener index for predicting the temperature at which paraffins boil [3]. Later, this measure became one of the most used descriptors and has found numerous applications, such as for the development of Quantitative Structure-Property (Structure-Activity) Relationships (QSPRs/QSARs) [2]. Many years after the introduction of the Wiener index and due to its success, an enormous number of other topological

indices have been put forward in the literature [4]. The most considered class of these graph invariants is distance-based topological indices, which are derived from the distance matrix or some related distance-based matrices [5], [6].

Many methods and algorithms for calculating distance-based topological indices were proposed in the literature. The complexity of these algorithms is overpowered by extracting and calculating all shortest paths [7]. An efficient algorithm was presented in [8] to reduce the computation of the Wiener index for benzenoid networks. Later, similar algorithms were developed for calculating some other topological indices [9]-[11].

In this research article, we concentrate on a recent topological index called the generalized Terminal Wiener index [12]. Our ultimate objective is to extend the method used in [8] and [13] to find the relation between the generalized Terminal Wiener index of a class of graphs, named partial cubes, and the Wiener index of weighted quotient graphs. Then, we prove that the application of this method on a partial cube named the graphenylene system can be implemented in linear time complexity. The graphenylene system is a two dimensional structure with an interesting topology, which was proposed by Balaban et al. [14] and is considered as a basis for nanostructural and electronic materials [15], [16]. The second objective of this work is to discuss and quantify the topological structure of two graphenylene networks, called the graphenylene chain network GC_n and the graphenylene sheet network GS_n .

The outline of this paper is organized as follows. In section 2, we give a general overview on the basic definitions and concepts that are required to present and prove the main results of this work. In section 3, we use the cut approach to calculate the generalized Terminal Wiener index of partial cubes. Then, we apply the main result to calculate the generalized Terminal Wiener index of graphenylene systems. Also, we show that the computation by using this technique can be done in $O(n)$ time complexity. In section 4, we give the construction method of the graphenylene chain network

GC_n and the graphylene sheet network GS_n . Furthermore, we apply the discussed linear method to find the generalized Terminal Wiener index of these structures. Finally, we recapitulate our findings in the last section.

2. PRELIMINARIES

Let $G = (V(G), E(G))$ be a connected graph, where $V(G)$ is the vertex set and $E(G)$ is the edge set of G . The distance $d_G(u, v)$ between two vertices u and v is defined as the number of edges in a shortest path from u to v in G . The notation $\deg(v)$ is the degree of a vertex v , which indicates the number of links incident to v . In the case of $\deg(v) = 1$, then the vertex v is a pendent vertex. A graph G is called a bipartite graph if the vertex set $V(G)$ can be divided into two disjoint sets $V_1(G)$ and $V_2(G)$ such that each edge in G must joins precisely one vertex of $V_1(G)$ to one vertex of $V_2(G)$. Let H be a subgraph of G , we say H is a convex subgraph of G if for any two vertices u and v in H , every shortest path between u and v in G lies completely to H . If $d_H(u, v) = d_G(u, v)$ for every two vertices u and v of H , then H is an isometric subgraph of G . The hypercube Q_n of dimension $n \geq 1$ is a graph constructed from a vertex set that are all binary strings of length n , such that two strings are adjacent if they differ in precisely one position. So, the category of partial cubes is constructed from isometric subgraphs of hypercubes Q_n . Let $e = xy$ and $f = uv$ be two edges that confirm the following relation:

$$d(x, u) + d(y, v) \neq d(x, v) + d(y, u).$$

Then, we state that e and f are in the relation *Djokovic-Winkler* Θ [17], [18]. The relation Θ is always reflexive symmetric, and transitive on partial cubes. Therefore, Θ partitions the edge set of a partial cube into equivalent classes $\{E_1, \dots, E_q\}$ called Θ classes or cuts. Now, we can note that G is a partial cube if and only if G is a bipartite graph and the components induced by $G - E_i$ are convex subgraphs of G . For more details on this category of graphs see [19].

In [3], the Wiener index of a graph G is defined as the sum of distances between all the vertices in G . Then

$$W(G) = \sum_{\{u,v\} \in V(G)} d_G(u, v). \tag{1}$$

For acyclic graphs T , the Wiener index can be calculated as:

$$W(T) = \sum_e n_1(e)n_2(e), \tag{2}$$

where $n_1(e)$ and $n_2(e)$ are the number of vertices of T located on the two sides of the edge e .

In [20], an extended version of the Wiener index for weighted graphs was proposed and formulated as follows. Let G be a graph and let $\omega: V(G) \rightarrow R$ be a weight function for the vertices of G . Then, the weighted Wiener index is defined as:

$$W(G, \omega) = \sum_{\{u,v\} \in V(G)} \omega(u)\omega(v)d_G(u, v). \tag{3}$$

Gutman et al. [21] introduced an extension of the Wiener index called the Terminal Wiener index and is defined as:

$$TW(G) = \sum_{\{u,v\} \in V_p(G)} d_G(u, v) \tag{4}$$

where $V_p(G)$ denotes the set of pendent vertices of the graph G .

Afterward, a generalization for the Terminal Wiener index was proposed in [12] and is defined as:

$$TW_K(G) = \sum_{\{u,v\} \in V_K(G)} d_G(u, v) \tag{5}$$

where $V_K(G)$ denotes the set of vertices with degree $K \geq 1$.

Toward more additional references on the Terminal Wiener index and its generalization, we refer to see [6], [22].

Now, we introduce the concept of the cut method, which is used as a tool to reduce the computation of the topological indices. The following theorem represents the first instance of this technique.

Theorem 1: [23] Let G be a partial cube and let $\{E_i\}_{i=1}^q$ be its Θ -classes. Let $n_1(E_i)$ and $n_2(E_i)$ be the number of vertices in the two connected components of $G - E_i$. Then

$$W(G) = \sum_{i=1}^q n_1(E_i)n_2(E_i). \tag{6}$$

The cut method for the generalized Terminal Wiener index reads as follows:

Theorem 2: Let G be a partial cube and $\{E_i\}_{i=1}^q$ be its Θ -partitions. Let $n_1^{(K)}(E_i)$ and $n_2^{(K)}(E_i)$ be the number of vertices of degree $K \geq 1$ in the two connected components of $G - E_i$. Then

$$TW_K(G) = \sum_{i=1}^q n_1^{(K)}(E_i)n_2^{(K)}(E_i). \tag{7}$$

Toward more results on the cut method, we refer to the papers [23]-[26].

3. A LINEAR METHOD FOR COMPUTING THE GENERALIZED TERMINAL WIENER INDEX OF GRAPHYLENE SYSTEMS

In this section, we prove the relation between the generalized Terminal Wiener index of partial cubes and the weighted Wiener index of quotient graphs. Then, we apply the obtained result to calculate the generalized Terminal Wiener index of graphylene systems and to prove that the computation can be done in $O(n)$ time complexity.

3.1 Generalized Terminal Wiener index of Partial Cubes

Let G be a partial cube and $\varepsilon = \{E_1, \dots, E_q\}$ be its Θ -classes.

The generalized Terminal Wiener index of G can be efficiently computed by applying the cut method, which was defined in **Theorem 2**. In the case of a huge partial cube G , the number of Θ -classes can be considerable. Based on this

limitation, we consider in the remaining of this study a partition $\{F_1, \dots, F_r\}$ of the set $E(G)$ coarser than ε such that F_i is the union of one or more Θ -classes of G . For proving our primary result, we have to introduce the notion of quotient graphs.

The quotient graph G/F_i , for $i \in \{1, \dots, r\}$, is a graph in which the vertices are the connected components of $G - F_i$. Two vertices C and C' in G/F_i being adjacent if there exist vertices $x \in C$ and $y \in C'$ such that $xy \in F_i$. Let $(G/F_i, \omega_i)$ be a weighted quotient graph, such that $\omega_i : V(G/F_i) \rightarrow N$ is the weight function that assigns to a vertex of G/F_i the number of vertices of degree K in the corresponding connected components of $G - F_i$. We note that we must consider only the vertices of degree K that already exist in the partial cube G .

Therefore, the computation of the generalized Terminal Wiener index can be reduced as follows:

Theorem 3: Let G be a partial cube with n vertices of degree K . Then

$$TW_K(G) = \sum_{i=1}^r W(G/F_i, \omega_i). \tag{8}$$

Proof:

Let α be the canonical metric representation of a partial cube G , such that α is defined as:

$$\alpha : G \rightarrow \prod_{1 \leq i \leq r} G/F_i$$

$$v \rightarrow (\alpha_1(v), \dots, \alpha_r(v))$$

where $\alpha_i(v)$ is the connected component of $G - F_i$ that contains the vertex v of degree K .

Let $C_1^{(i)}, \dots, C_{s_i}^{(i)}$ be the connected components of $G - F_i$ and $|V_K(C_j^{(i)})|$ be the number of vertices with degree K in the component $C_j^{(i)}$. We note that $\sum_{j=1}^{s_i} |V_K(C_j^{(i)})| = n$.

Let $P_{u,v}$ be the shortest path between $u, v \in V_K(G)$. We can verify that $|E(P_{u,v}) \cap F_i| = 0$ if u, v belong to the same component $C_j^{(i)}$, otherwise $|E(P_{u,v}) \cap F_i| \neq 0$.

Let $C_j^{(i)}$ and $C_{j'}^{(i)}$ be two connected components of $G - F_i$. To be specific, $C_j^{(i)}$ and $C_{j'}^{(i)}$ are two vertices of G/F_i . Let $u, u' \in V(C_j^{(i)})$ and $v, v' \in V(C_{j'}^{(i)})$. Then, we can see that $|E(P_{u,v}) \cap F_i| = |E(P_{u',v'}) \cap F_i|$ (for more details, see [13]).

This observation yields to:

$$d_{G/F_i}(C_j^{(i)}, C_{j'}^{(i)}) = |E(P_{u,v}) \cap F_i|.$$

We define a function $\delta : V(G) \rightarrow \{0,1\}$ as follows:

$$\delta(P_{u,v}) = \begin{cases} 0; & \text{if } u, v \in C_p^{(i)} \\ 1; & \text{if } u \in C_p^{(i)} \text{ and } v \in C_{p'}^{(i)} \end{cases}$$

The summation $\sum_{u,v \in V_K(G)} \delta(P_{u,v})$ is equal to the number of times that we pass through the edges of F_i . Thus:

$$\sum_{u,v \in V_K(G)} \delta(P_{u,v}) = \sum_{1 \leq j < j' \leq s_i} |V_K(C_j^{(i)})| |V_K(C_{j'}^{(i)})|$$

From the above notations and the canonical metric representation α , we can see that:

$$\begin{aligned} TW_K(G) &= \sum_{\{u,v\} \in V_K(G)} d_G(u,v) \\ &= \sum_{\{u,v\} \in V_K(G)} d_G(\alpha(u), \alpha(v)) \\ &= \sum_{\{u,v\} \in V_K(G)} \sum_{i=1}^r d_{G/F_i}(\alpha_i(u), \alpha_i(v)) \\ &= \sum_{\{u,v\} \in V_K(G)} \sum_{i=1}^r |E(P_{u,v}) \cap F_i| \\ &= \sum_{i=1}^r \sum_{\{u,v\} \in V_K(G)} |E(P_{u,v}) \cap F_i| \\ &= \sum_{i=1}^r \sum_{1 \leq j < j' \leq s_i} |V_K(C_j^{(i)})| |V_K(C_{j'}^{(i)})| d_{G/F_i}(C_j^{(i)}, C_{j'}^{(i)}) \\ &= \sum_{i=1}^r W(G/F_i, \omega_i). \end{aligned}$$

The proof is complete.

3.2 Generalized Terminal Wiener index of Graphenylene Systems

Graphenylene systems are connected graphs constructed in the following manner. Let \mathbb{H} be a semiregular (4.6.12)-tiling lattice, such that there is one square C_4 , one hexagon C_6 and one dodecagon C_{12} on each vertex. Let Z be a circuit on \mathbb{H} . Then, a graphenylene system is formed by the vertices and the edges of \mathbb{H} lying on Z and in its interior. **Figure 1** illustrates the construction method of a graphenylene system. It was proved in [27] that all connected subgraphs of (4.6.12)-tiling lattice are partial cubes. Thus, each graphenylene system is a partial cube.

Let G be a graphenylene system and $\{E_1, \dots, E_q\}$ be its Θ -classes. From the construction method of a graphenylene system, we can see that G contains a dodecagon C_{12} , which holds six different directions of edges, see **Figure 2**. Therefore, $\{F_1, F_2, \dots, F_6\}$ is a partition coarser than Θ -classes, where each F_i is the union of all Θ -partitions with the same direction. Let G/F_i be the quotient graph whose vertices are the connected components of $G - F_i$, $i \in \{1, 2, \dots, 6\}$, and let $(G/F_i, \omega_i)$ be the weighted quotient graphs that are constructed as illustrated in the previous subsection 3.1. The following fundamental result is a special case of the Theorem 3.

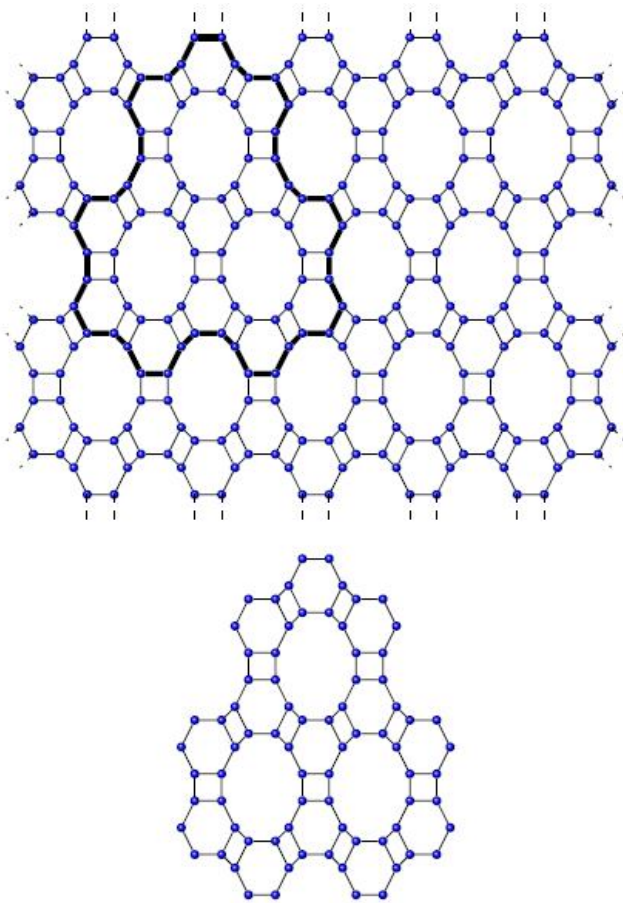


Figure 1: (Top) The (4.6.12)-tiling lattice H and the circuit Z . (Bottom) A graphenylene system G .

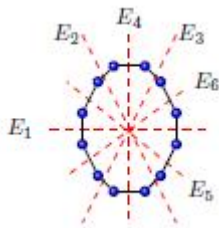


Figure 2: The six different directions of elementary cuts $E_i, i \in \{1, 2, \dots, 6\}$.

Corollary 1: Let G be a graphenylene system and $\{F_i\}_{i=1}^6$ be a partition coarser than Θ -classes. Then

$$TW_K(G) = \sum_{i=1}^6 W(G/F_i, \omega_i). \tag{9}$$

The final step in this subsection is to prove that the generalized Terminal Wiener index of a graphenylene system G can be computed in linear time. At first, we have to show that each quotient graph G/F_i is a tree, with $i \in \{1, 2, \dots, 6\}$.

Lemma 1: Let G be a graphenylene system and $\{F_i\}_{i=1}^6$ be a partition coarser than Θ -classes. Then, each quotient graph G/F_i is a tree, for $i \in \{1, 2, \dots, 6\}$.

Proof: Let suppose that G/F_i is not a tree and obviously contains a cycle. This implies that G must contain an interior face different than a square C_4 , a hexagon C_6 and a

dodecagon C_{12} . From this contradiction, there is no cycle in G/F_i and therefore, G/F_i is a tree.

We recall from [28] that the weighted quotient trees $(G/F_i, \omega_i)$ can be obtained in linear time. In [8], it was proved that the Wiener index of a weighted tree (T, ω) is given by:

$$W(T, \omega) = \sum_{e \in E(T)} n_1(e)n_2(e), \tag{10}$$

where $n_i(e) = \sum_{u \in T-e} \omega(u), \text{ for } i = 1, 2.$

By using equation 10 the Wiener index of a weighted tree $(G/F_i, \omega_i)$ is calculated in $O(n)$ time. Finally, we get the following primary result.

Theorem 4: If G is a graphenylene system with n vertices, then the generalized Terminal Wiener index can be computed in $O(n)$ time.

The computation in linear time is possible for some other systems that full under partial cubes, such as square systems, hexagonal systems and C_4C_8 systems. In [10], it was proved that the Wiener index and the Szeged index of C_4C_8 systems can be computed in linear time. Therefore, we report the following generalization.

Corollary 2: If G is a system with a fixed number of Θ -classes that have the same direction, and all the corresponding quotient graphs are trees. Then, the generalized Terminal Wiener index can be computed in linear time.

4. QUANTIFYING THE TOPOLOGICAL STRUCTURE OF GRAPHENYLENE NETWORKS

In this section, we discuss two graphenylene networks called graphenylene chain network GC_n and graphenylene sheet network GS_n . At first, we present the construction method of these two structures. Then, we apply the linear method to find exact analytical expression for the generalized Terminal Wiener index of graphenylene chain networks GC_n and graphenylene sheet networks GS_n .

4.1 Graphenylene Chain Network

Let HS_n be a hexagonal-square chain of dimension n , which is obtained by alternating C_6 and C_4 . The graph HS_n contains $2n+1$ hexagon C_6 and $2n$ square C_4 . Thus, the graphenylene chain network GC_n of dimension n is obtained by joining two hexagonal-square chains of dimension n . The construction method of a graphenylene chain network is illustrated in **Figure 3**. The number of vertices of GC_n is equal to $24n+12$.

Now, we apply the linear method in order to obtain exact formula for the generalized Terminal Wiener index of the graphenylene chain network GC_n . We consider the case of K equals to the maximum degree Δ . From **Figure 3**, we can

observe that $\Delta = 3$ and the number of vertices of degree 3 is equal to: $N_\Delta = 20n + 4$.

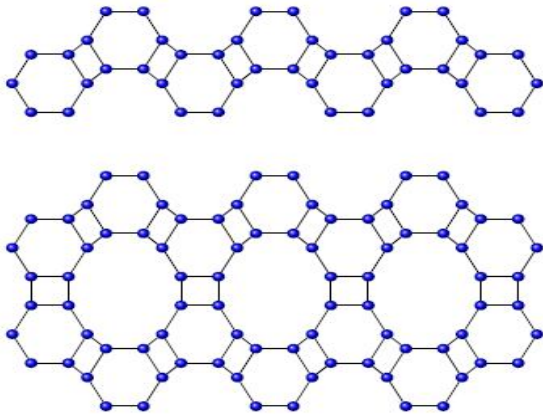


Figure 3: The construction method of a graphenylene chain network of dimension 3. (Top) A hexagonal-square chain HS_3 . (Bottom) A graphenylene chain network GC_3 .

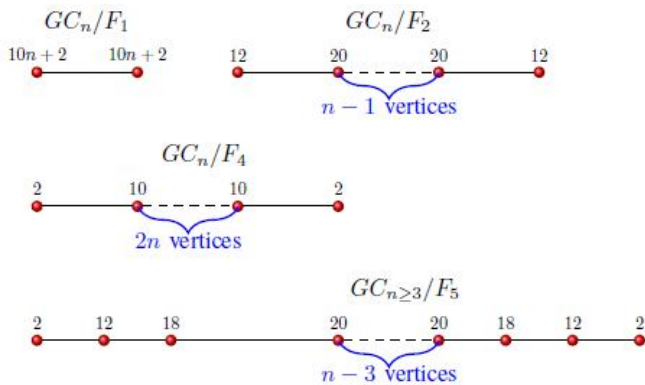
Theorem 5:

Let GC_n be a graphenylene chain network of dimension $n \geq 2$. Then,

$$TW_\Delta(GC_n) = 400n^3 + 340n^2 + 524n - 152. \quad (11)$$

Proof: The graphenylene chain network GC_n is a partial cube and holds six different directions of edges, as shown in Figure 2. First, for $i \in \{1,2,\dots,6\}$, we determine the components $GC_n - F_i$, where F_i is the union of the elementary cuts with the same direction i .

Then, we get the following weighted quotient trees $(GC_n / F_i, \omega_i)$, for $i = \{1,2,\dots,6\}$ and $n \geq 2$.



$$\begin{aligned} W(GC_n / F_4, \omega_4) &= \sum_{i=0}^{2n} (2 + 10i) * [N_\Delta - (2 + 10i)] \\ &= \frac{400}{3} n^3 + 80n^2 + \frac{44}{3} n + 4. \\ W(GC_n / F_5, \omega_5) &= 2 * [2 * (N_\Delta - 2) + 14 * (N_\Delta - 14)] + \\ &\quad \sum_{i=0}^{n-3} (32 + 20i) * [N_\Delta - (32 + 20i)] \\ &= \frac{200}{3} n^3 + 40n^2 + \frac{592}{3} n - 80. \end{aligned}$$

Clearly, we have $W(GC_n / F_2, \omega_2) = W(GC_n / F_3, \omega_3)$ and $W(GC_n / F_5, \omega_5) = W(GC_n / F_6, \omega_6)$. Thus, from the application of Corollary 1, we get the result.

We show in **Figure 4** the performance of the generalized Terminal Wiener index of the Graphenylene chain network GC_n . In the horizontal and the vertical axis, we have the dimension n and the values of the generalized Terminal Wiener index of GC_n , respectively. From this graphical representation, we can see that the value of the generalized Terminal Wiener index increases with the growth of the dimension n and approximates to $400n^3$ if the dimension n gets large enough.

Due to the symmetry in GC_n network, the weighted quotient tree GC_n / F_3 is isomorphic to GC_n / F_2 and GC_n / F_6 is isomorphic to GC_n / F_5 .

Next, we calculate the Weighted Wiener index of quotient trees GC_n / F_i , for $i = \{1,2,\dots,6\}$, by using the Equation 10.

$$\begin{aligned} W(GC_n / F_1, \omega_1) &= 100n^2 + 40n + 4 \\ W(GC_n / F_2, \omega_2) &= \sum_{i=0}^{n-1} (12 + 20i) * [N_\Delta - (12 + 20i)] \\ &= \frac{200}{3} n^3 + 40n^2 + \frac{112}{3} n \end{aligned}$$

Figure 4: The graphical behavior of the generalized Terminal Wiener index of the graphenylene chain network GC_n .

4.2 Graphenylene Sheet Network

Let GS_n be a graphenylene sheet network of dimension n , where n denotes the number of dodecagon C_{12} in each side of this network. The GS_n can be obtained by joining n graphenylene chain networks of dimension n . An example of a graphenylene sheet network is shown in **Figure 5**. The number of vertices of GS_n is $12n^2 + 16n - 4$.

Now, we calculate the generalized Terminal Wiener index of the graphenylene sheet network GS_n in the case of $K = \Delta$. From **Figure 5**, we can see that the number of vertices of degree Δ is equal to: $N_\Delta = 12n^2 + 16n - 4$.

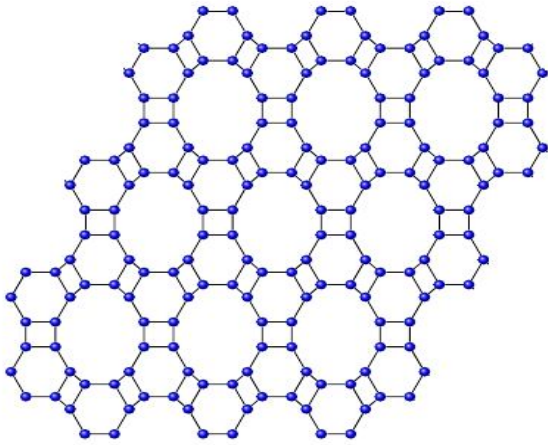
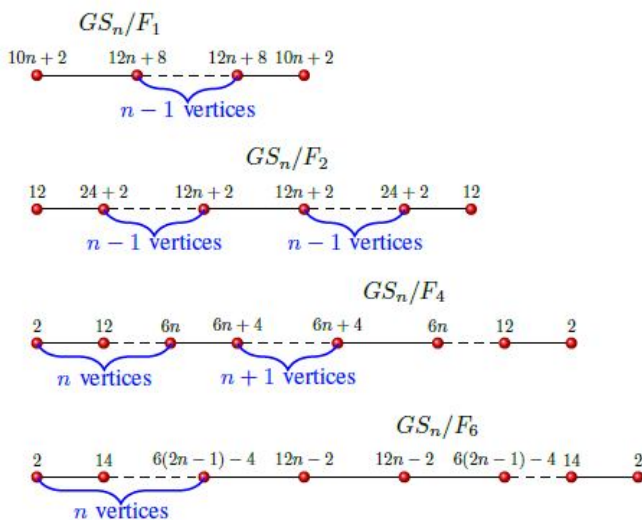


Figure 5: A graphenylene sheet network GS_n of dimension $n=3$.

Theorem 6: Let GS_n be a graphenylene sheet network of dimension $n \geq 2$. Then,

$$TW_{\Delta}(GS_n) = 222n^5 + 740n^4 + \frac{1102}{3}n^3 - 252n^2 + \frac{152}{3}n. \tag{12}$$

Proof: The graphenylene sheet network GS_n is a partial cube and holds six different directions of edges, as illustrated in **Figure 2**. The calculation process of the generalized Terminal Wiener index TW_{Δ} of GS_n is similar to that for GC_n . At first, we determine the components $GS_n - F_i$, where F_i is the union of the elementary cuts with the same direction i . Then, we construct the weighted quotient trees $(GS_n / F_i, \omega_i)$, for $i = \{1, 2, \dots, 6\}$ and $n \geq 2$, which are defined as follows:



Due to the symmetry of the GS_n network, the weighted quotient tree GS_n / F_3 is isomorphic to GS_n / F_1 and GS_n / F_5 is isomorphic to GS_n / F_4 .

Now, we calculate the Weighted Wiener index of quotient trees GS_n / F_i , for $i = \{1, 2, \dots, 6\}$, by using the Equation 10.

$$W(GS_n / F_1, \omega_1) = \sum_{i=0}^{n-1} [(10n+2) + (12n+8)i]^* [N_{\Delta} - [(10n+2) + (12n+8)i]].$$

$$W(GS_n / F_2, \omega_2) = 2 \left(\sum_{i=2}^{n-1} \left[12 + \sum_{j=2}^i (12j+2) \right]^* \left[N_{\Delta} - \left[12 + \sum_{j=2}^i (12j+2) \right] \right] \right) + \left[\frac{N_{\Delta}}{2} \right]^2 + 24[N_{\Delta} - 12].$$

$$W(GS_n / F_4, \omega_4) = 4[N_{\Delta} - 2] + 2 \left(\sum_{i=2}^n \left[2 + \sum_{j=2}^i 6i \right]^* \left[N_{\Delta} - \left[2 + \sum_{j=2}^i 6i \right] \right] \right) + \sum_{i=1}^n \left[2 + \sum_{i=2}^n 6i + (6n+4)i \right].$$

$$W(GS_n / F_6, \omega_6) = 2 \left(\sum_{i=0}^{n-1} \left[\sum_{j=0}^i (6(2i+1) - 4) \right]^* \left[N_{\Delta} - \left[\sum_{j=0}^i (6(2i+1) - 4) \right] \right] \right) + \left(\frac{N_{\Delta}}{2} \right)^2.$$

Obviously, we have $W(GS_n / F_1, \omega_1) = W(GS_n / F_3, \omega_3)$ and $W(GS_n / F_4, \omega_4) = W(GS_n / F_5, \omega_5)$. Finally, we apply the Corollary 1 in order to get the result.

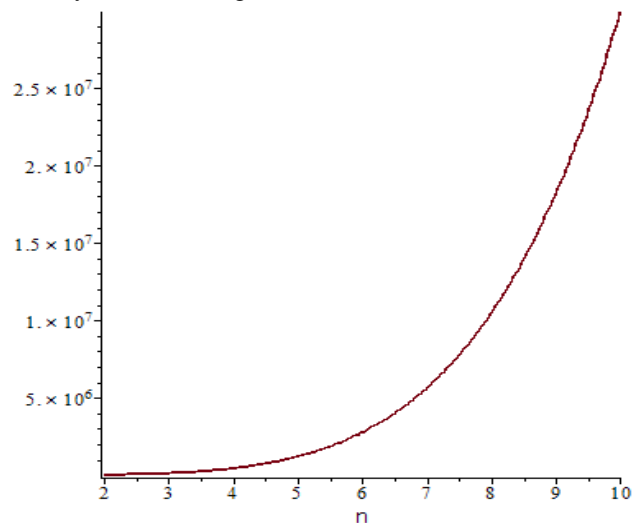


Figure 6: The graphical behavior of the generalized Terminal Wiener index of the graphenylene sheet network GS_n .

We show in **Figure 6** the performance of the generalized Terminal Wiener index of the Graphenylene sheet network GS_n . In the horizontal axis, we have the dimension n and in the vertical axis the values of the generalized Terminal Wiener index of GS_n are determined. From this graphical representation, we observe that the value of the generalized Terminal Wiener index shows a dominant change with the increase of the dimension n and approximates to $222n^5$ if the dimension n gets large enough.

5. CONCLUSION

In this manuscript, we studied the computation efficiency of the generalized Terminal Wiener index of partial cubes. Then, we applied the obtained result to calculate the generalized Terminal Wiener index of graphenylene systems in linear time complexity. Also, we showed that the main result is an efficient tool to quantify the topological structure of two graphenylene systems called the graphenylene chain network GC_n and the graphenylene sheet network GS_n . For these networks, we calculated the generalized Terminal Wiener index in the case of K equals to the maximum degree. The out-findings of this paper are novel and play a significant role to figure out the structural properties of graphenylene networks. Also, they are considered as an eye-opener for researchers working in different fields such as computer science, nanoscience and network science.

REFERENCES

1. M. Knor, R. Skrekovski, **Wiener index of line graphs**. *Quantitative Graph Theory: Mathematical Foundations and Applications*, pp. 279-301, 2014. <https://doi.org/10.1201/b17645-10>
2. J. Devillers, A. T. Balaban, **Topological Indices and Related Descriptors in QSAR and QSPR**. *Gordon and Breach Science Publishers, Amsterdam, the Netherlands*, 2000.
3. H. Wiener, **Structural determination of paraffin boiling points**. *Journal of the American Chemical Society*, Vol. 69, pp. 17-20, 1947. <https://doi.org/10.1021/ja01193a005>
4. R. Todeschini, V. Consonni, **Molecular Descriptors for Chemoinformatics**. *Wiley-VCH, Weinheim, Germany*, 2009. <https://doi.org/10.1002/9783527628766>
5. Z. Mihalic, S. Nikolic, N. Trinajstic, **Comparative study of molecular descriptors derived from the distance matrix**. *Journal of Chemical Information and Computer Sciences*, Vol. 32, no. 1, pp. 28-37, 1992. <https://doi.org/10.1021/ci00005a005>
6. K. Xu, M. Liu, K. C. Das, I. Gutman, B. Furtula, **A survey on graphs extremal with respect to distance-based topological indices**. *MATCH Commun. Math. Comput. Chem*, Vol. 71, no. 3, pp. 461-508, 2014.
7. B. Mohar, T. Pisanski, **How to compute the Wiener index of graph**. *Journal of Mathematical Chemistry*, Vol. 2, no. 3, pp. 267-277, 1988. <https://doi.org/10.1007/BF01167206>
8. V. Chepoi, S. Klavzar, **The wiener index and the Szeged index of benzenoid systems in linear time**. *Journal of chemical information and computer sciences*. Vol. 37, pp. 752-755, 1997. <https://doi.org/10.1021/ci9700079>
9. A. Kelenc, S. Klavzar, N. Tratnik, **The edge-Wiener index of benzenoid systems in linear time**. *MATCH Commun. Math. Comput. Chem*, Vol. 74, no.3, pp. 521-532, 2015.
10. M. Crepnjak, N. Tratnik, **The Szeged index and the Wiener index of partial cubes with applications to chemical graphs**. *Applied Mathematics and Computation*. Vol. 309, pp. 324-333, 2017. <https://doi.org/10.1016/j.amc.2017.04.011>
11. N. Tratnik, **The edge-Szeged index and the PI index of benzenoid systems in linear time**. *MATCH Commun. Math. Comput. Chem*, Vol. 77, pp. 393-406, 2017.
12. A. Ilic, M. Ilic, **Generalizations of Wiener polarity index and terminal Wiener index**. *Graphs and Combinatorics*, Vol. 29, no. 5, pp. 1403-1416, 2013. <https://doi.org/10.1007/s00373-012-1215-6>
13. S. Klavzar, M. J. Nadjafi-Arani, **Wiener index in weighted graphs via unification of θ^* -classes**. *European Journal of Combinatorics*. Vol. 36, pp. 71-76, 2014. <https://doi.org/10.1016/j.ejc.2013.04.008>
14. A. T. Balaban, K. P. C. Vollhardt, **Heliphenes and Related Structures**. *The Open Organic Chemistry Journal*, Vol. 5, no.1, 2011. <https://doi.org/10.2174/1874364101105010117>
15. A. T. Koch, A. H. Khoshaman, H. D. Fan, G. A. Sawatzky, A. Nojeh, **Graphenylene nanotubes**. *The journal of physical chemistry letters*, Vol. 6, no. 19, pp. 3982-3987, 2015. <https://doi.org/10.1021/acs.jpcclett.5b01707>
16. J. M. Schulman, R. L. Disch, **A theoretical study of large planar [N] phenylenes**. *The Journal of Physical Chemistry A*, Vol. 111, no. 39, pp. 10010-10014, 2007. <https://doi.org/10.1021/jp074454v>
17. D. Djokovic, **Distance preserving subgraphs of hypercubes**. *Journal of Combinatorial Theory, Series B*, Vol. 14, no. 263-267, 1973. [https://doi.org/10.1016/0095-8956\(73\)90010-5](https://doi.org/10.1016/0095-8956(73)90010-5)
18. P. Winkler, **Isometric embeddings in products of complete graphs**. *Discrete Applied Mathematics*, Vol. 7, pp. 221-225, 1984. [https://doi.org/10.1016/0166-218X\(84\)90069-6](https://doi.org/10.1016/0166-218X(84)90069-6)
19. R. Hammack, W. Imrich, S.K. Klavzar, **Handbook of Product Graphs**. *second ed., CRC Press, Taylor & Francis Group, Boca Raton*, 2011. <https://doi.org/10.1201/b10959>
20. S. Klavzar, I. Gutman, **Wiener number of vertex-weighted graphs and a chemical application**. *Discrete Applied Mathematics*, Vol. 80, pp.73-81, 1997. [https://doi.org/10.1016/S0166-218X\(97\)00070-X](https://doi.org/10.1016/S0166-218X(97)00070-X)
21. I. Gutman, B. Furtula, M. Petrovic, **Terminal wiener index**. *Journal of mathematical chemistry*, Vol. 46, pp. 522-531, 2009. <https://doi.org/10.1007/s10910-008-9476-2>
22. M. Zeryouh, M. El Marraki, M. Essalih, **On the Terminal Wiener index of networks**. *In Multimedia Computing and Systems (ICMCS), 2016 5th International Conference on, IEEE*, pp. 533-536, 2016. <https://doi.org/10.1109/ICMCS.2016.7905645>
23. S. Klavzar, **A bird's eye view of the cut method and a survey of its applications in chemical graph theory**.

- MATCH Commun. Math. Comput. Chem.* Vol. 60, no. 2, pp. 255-274, 2008.
24. S. Klavzar, M. J. Nadjafi-Arani, **Cut method: update on recent developments and equivalence of independent approaches.** *Current Organic Chemistry*, Vol. 19, no. 4, pp. 348-358, 2015.
<https://doi.org/10.2174/1385272819666141216232659>
25. M. Zeryouh, M. El Marraki, M. Essalih, **Studying the Structure of Some Networks Using Certain Topological Indices.** In *International Workshop on Complex Networks and their Applications*. Springer, Cham, pp. 543-554, 2017.
https://doi.org/10.1007/978-3-319-72150-7_44
26. M. Arockiaraj, S. R. J. Kavitha, K. Balasubramanian, **Vertex cut method for degree and distance-based topological indices and its applications to silicate networks.** *Journal of Mathematical Chemistry*, Vol. 54, no. 8, pp. 1728-1747, 2016.
<https://doi.org/10.1007/s10910-016-0646-3>
27. Y. J. Pan, M. F. Xie, F. J. Zhang, **Partial Cubes and Archimedean Tilings.** *Acta Mathematicae Applicatae Sinica, English Series*, Vol. 34, no. 4, pp. 782-791, 2018.
<https://doi.org/10.1007/s10255-018-0788-0>
28. V. Chepoi, **On distances in benzenoid systems.** *Journal of Chemical Information and Computer Sciences*. Vol. 36, pp. 1169-1172, 1996.
<https://doi.org/10.1021/ci9600869>