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A STUDY ON THE MINIMUM DEGREE WIENER INDEX OF GRAPHS †

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ABSTRACT. In this paper, we introduced a new distance-based index called the minimum degree Wiener index, which is the sum of distances between all unordered pairs of vertices with the minimum degree. Additionally, a matrix related to this index was introduced, and it was discovered that the sum of entries in each row was the same for some classes of graphs, contrary to many graph-related matrices. In particular, we determined the minimum degree Wiener index of the bipartite Kneser graph, bipartite Kneser type-k graphs, Johnson graph and the set inclusion graphs. The terminal Wiener index of a graph G is the sum of distances between all unordered pairs of pendant vertices of G. Also, we determined Wiener index, hyper Wiener index and corresponding polynomials of the bipartite Kneser type-k graphs for k = 2, 3.

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1. Introduction

In the chemical sciences as well as pharmaceuticals, graph theory is a crucial tool for understanding diverse algebraic structures and molecular properties. We are able to generate a molecular graph from a molecule by representing the atoms as vertices and the bonds as edges. Topological indices [15],[6] are graph theoretic invariants of molecular graphs which predict the characteristics of the related molecule. A simple graph G = (V, E) consists of a vertex set V and an edge set E, where each edge in E connects two distinct vertices in V. The number of vertices, |V|, is the order of the graph G and the number of edges,

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|E|, is the size of the graph G. Degree of a vertex v in a simple graph denoted by d(v) is the number of edges incident on it. A vertex v is a cut vertex of a connected graph G if G - v is disconnected. A graph G is a 2-connected graph if it contains no cut vertices [10],[16]. In a molecular graph, vertices represent carbon atoms, edges represent the bonds between the atoms, and degree of a vertex denotes the valency.

In a bipartite graph, the set of vertices is divided into two disjoint subsets and every edge connects a vertex from one of these subsets to a vertex from the other subset. The graph invariants of bipartite graphs are very useful in transportation problems, coding theory, etc. [2], [4]. Kneser graphs are defined as graphs with k-element subsets of a fixed set with n elements as vertices, and the adjacency exists between two disjoint k-element subsets [11]. The bipartite Kneser graph H(n,k) [13] for a positive integer n > 1 has a vertex set consisting of all k-element and n-k element subsets of $S_n = \{1, 2, 3, ..., n\}$, and an edge between any two vertices U and W exists when $U \subset W$ or $W \subset U$. For an integer $k, 1 \leq k \leq n-1$, the bipartite Kneser type-k graph $H_T(n,k)$ [19], was defined as a graph with partition (V_1, V_2) in which V_1 contains k-element subsets of S_n , n > 1, and V_2 contains all non-empty subsets of S_n which are not in V_1 . Define the edge set as $\{UW : U \in V_1, W \in V_2, \text{ and } UW \text{ exists if and only if } U \subset W \text{ or } W \subset U\}.$ The bipartite Kneser type-1 graph and some of its properties were established in [18]. In [17], it is shown that the graphs $H_T(n,k)$ and $H_T(n,n-k)$ are isomorphic for all n and k. The connectivity and diameter of the graph $H_T(n,k)$ were also discussed.

The Wiener index of a graph G, W(G), the most well-known distance-based index, was introduced by Harold Wiener in 1947 and is defined as the total distance between unordered pairs of vertices in a graph [5]. Further Wiener introduced Wiener polarity index $W_p(G)$ of a graph G, [1], as the number of unordered pairs of vertices that are at distance 3 in G. In [7] and [8], the terminal Wiener index was introduced in connection with the terminal distance matrix, which was used in genetic codes, and in mathematical modelling of proteins [9], [14].

In this paper, we discussed Wiener and hyper-Wiener indices, which are distance-based topological indices, of the graphs $H_T(n, 2)$ and $H_T(n, 3)$. A new, graph topological index called the minimum degree Wiener index was introduced, along with a related polynomial. In addition, a matrix associated with this index was established, and it was shown that, in contrast to many graph-related matrices, the sum of entries in each row was the same for some classes of graphs. We computed these indices for bipartite Kneser graph, bipartite Kneser type-k graphs, Johnson graphs, set inclusion graphs.

2. Preliminaries

Throughout this paper, we consider only simple connected graphs unless otherwise mentioned. The distance (that is, the length of a shortest path) between any two distinct vertices u and v is denoted by d(u, v). In a graph G, the minimum degree among the vertices of G is denoted by $\delta(G)$ and the maximum degree of G is denoted by $\Delta(G)$.

Definition 2.1. [19] Let $S_n = \{1, 2, 3, ..., n\}$, n > 1 and $1 \le k < n$. The bipartite Kneser type-k graph is defined as a bipartite graph with partition (V_1, V_2) in which V_1 contains k-element subsets of S_n , and V_2 contains all other non-empty subsets of S_n , and is denoted by $H_T(n, k)$. The adjacency of $H_T(n, k)$ is defined as: two vertices $U \in V_1$, $W \in V_2$ are adjacent if and only if either $U \subset W$ or $W \subset U$.

In V_1 , all the vertices have the same degree $2^k + 2^{n-k} - 3$. In V_2 , $\binom{n}{i}$ vertices have degrees $\binom{n-i}{k-i}$, where $i \in \{1, 2, 3, \ldots, k-1\}$ and $\binom{n}{j}$ vertices have degrees $\binom{j}{k}$, where $j \in \{k+1, k+2, \ldots, n-1\}$.

The previous studies in [17] showed that the diameter of the graph $H_T(n, k)$ for $n > 3, 1 \le k < n$ is 4 and, the vertex connectivity and the edge connectivity are k + 1. If a graph's vertex connectivity is greater than or equal to 2, then it is said to be 2-connected. So $H_T(n, k)$ graphs for n > 3 are 2-connected.

Theorem 2.2. [10] Let G be a 2-connected graph of order ω . Then

$$W(G) \leq \begin{cases} \frac{\omega^3}{8} & \text{if } \omega \text{ is even}, \\ \frac{\omega(\omega-1)(\omega+1)}{8} & \text{if } \omega \text{ is odd}, \end{cases}$$

equality holds if and only if $G \cong C_{\omega}$, where C_{ω} is the cycle graph with ω vertices.

3. Main results

3.1. Minimum degree Wiener index. The sum of the distances between all unordered pairs of pendant vertices on a graph G is the terminal Wiener index of that graph [8]. Motivated from the concept of terminal Wiener index, we introduce a new distance related topological index called minimum degree Wiener index, MDW(G) of a graph G as follows:

Definition 3.1. Let G be a simple connected graph. Let $V_{min} = \{U_i \in V(G) : d(U_i) = \delta\}$. Define the minimum degree Wiener index MDW(G) of G as $MDW(G) = \sum_{U_i, U_j \in V_{min}} d(U_i, U_j)$ for all unordered pairs of vertices (U_i, U_j) .

Observation 1.

- For trees, the minimum degree Wiener index and the terminal Wiener index are the same.
- If there is only one vertex with minimum degree, then MDW(G) = 0.
- If the graph has exactly two vertices U_1, U_2 with minimum degree, then $MDW(G) = d(U_1, U_2)$.
- If there exist exactly two vertices U_1, U_2 with minimum degree and have same adjacent vertex, then MDW(G) = 2.

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• For regular graphs, the minimum degree Wiener index and the Wiener index are the same.

Here we discuss the minimum degree Wiener index of the bipartite Kneser type-k graphs. Let us consider an example: $H_T(4, 2)$:

FIGURE 1. The graph of $H_T(4,2)$



From the Definition 2.1, the vertices of $H_T(4,2)$ represent as follows: 1 = $\{1,2\}, 2 = \{1,3\}, 3 = \{1,4\}, 4 = \{2,3\}, 5 = \{2,4\}, 6 = \{3,4\}, 7 = \{1\}, 8 = \{1,2\}, 1 = \{1,3\}, 1 =$ $\{2\}, 9 = \{3\}, 10 = \{4\}, 11 = \{1, 2, 3\}, 12 = \{1, 2, 4\}, 13 = \{1, 3, 4\}, 14 = \{1, 2, 3\}, 12 = \{1, 2, 4\}, 13 = \{1, 3, 4\}, 14 =$ $\{2,3,4\}, 15 = \{1,2,3,4\}$

Here $V_{min} = \{7, 8, 9, 10, 11, 12, 13, 14\}.$

$$MDW(H_T(4,2)) = d(7,8) + d(7,9) + d(7,10) + d(7,11) + d(7,12) + d(7,13) + d(7,14) + d(8,9) + d(8,10) + d(8,11) + d(8,12) + d(8,13) + d(8,14) + d(9,10) + d(9,11) + d(9,12) + d(9,13) + d(9,14) + d(10,11) + d(10,12) + d(10,13) + d(10,14) + d(11,12) + d(11,13) + d(11,14) + d(12,13) + d(12,14) + d(13,14) = 64.$$

Observation 2.

- For bipartite Kneser type-k graphs $H_T(n,k)$, the minimum degree δ is
- k+1.• For $1 \le k \le \lfloor \frac{n}{2} \rfloor$ and $k \ne \frac{n}{2}$, the number of minimum degree vertices, $|V_{min}| = \binom{n}{k+1}.$

• For
$$1 \le k \le \left\lfloor \frac{n}{2} \right\rfloor$$
 and $k = \frac{n}{2}$, $|V_{min}| = \binom{n}{k-1} + \binom{n}{k+1}$.

We define a restricted distance matrix of a graph G as $MDM(G) = [U_{ij}]$,

where $U_{ij} = \begin{cases} d(U_i, U_j) & if \quad U_i, U_j \in V_{min} \\ 0 & \text{otherwise.} \end{cases}$

This matrix is a real symmetric matrix with 0 as diagonal elements. Order of the matrix is |V(G)|.

Now we construct a matrix by indexing the rows and columns with the vertex subset V_{min} of G. This matrix called **minimum** δ -distance matrix of a graph G, and is defined as follows:

Let G be a graph with |V(G)| = n. If G has m vertices with minimum degree, and these m vertices are labeled as U_1, U_2, \ldots, U_m , then its minimum δ -distance matrix is the square matrix of order m whose $(i, j)^{th}$ – entry is $d(U_i, U_j)$. That is, $M_{\delta}DM(G) = [U_{ij}]$, where $U_{ij} = d(U_i, U_j), U_i, U_j \in V_{min}$. This is also a real symmetric matrix with all diagonal entries 0.

Theorem 3.2. Let G be a 2-connected graph of order $\omega \geq 4$. Then

$$0 \leq MDW(G) \leq \begin{cases} \frac{\omega^3}{8} & \text{if } \omega \text{ is even,} \\ \\ \frac{\omega(\omega-1)(\omega+1)}{8} & \text{if } \omega \text{ is odd.} \end{cases}$$

Proof. By the definition of minimum degree Wiener index, $MDW(G) \leq W(G)$. If $|V(G)| = |V_{min}|$, then MDW(G) = W(G). If there is only one vertex with minimum degree, that is, if $|V_{min}| = 1$, MDW(G) = 0. Thus $MDW(G) \ge 0$. Hence by Theorem 2.2, we have the result. \square

Theorem 3.3. For the graph $H_T(n,k)$, where n > 3, $1 \le k \le \left\lfloor \frac{n}{2} \right\rfloor$ and $k \ne \frac{n}{2}$, we have

$$MDW(H_T(n,k)) = \binom{n}{k+1} \left\{ (n-k-1)(k+1) + 2\left[\binom{n-k-1}{k+1} + \sum_{i=1}^{k-1} \binom{k+1}{i} \binom{n-k-1}{k+1-i}\right] \right\}.$$

Proof. By Definition 2.1, the minimum degree vertices occur in the part V_2 . The distance between any two vertices in V_2 is either 2 or 4. Using the minimum below the formation of the vertices in V_2 is other 2 of N compared minimum δ -distance matrix, in each row, the number of unordered pairs of vertices in V_2 with distance 2 is $\binom{k+1}{k}\binom{n-(k+1)}{k+1-k} = (n-k-1)(k+1)$ and those with distance 4 is $\binom{n-k-1}{k+1} + \sum_{i=1}^{k-1} \binom{k+1}{i}\binom{n-k-1}{k+1-i}$. Thus the minimum degree Wiener index

is given by

$$MDW(G) = \frac{\binom{n}{k+1}}{2} \left\{ 2(n-k-1)(k+1) + 4 \left[\binom{n-k-1}{k+1} + \sum_{i=1}^{k-1} \binom{k+1}{i} \binom{n-k-1}{k+1-i} \right] \right\}.$$
 nce the result.

Hence the result.

Theorem 3.4. For the bipartite Kneser type-k graphs $H_T(n,k)$, where $k = \frac{n}{2}, n \neq 4$,

$$MDW(H_T(n,k)) = \frac{\binom{n}{k-1} + \binom{n}{k+1}}{2} \left[2 \ d(G,2) + 4 \ d(G,4) \right],$$

where d(G, 2) = (k - 1)(n - k + 1) + (k + 1) and $d(G, 4) = \binom{n - k + 1}{k - 1} + \sum_{i=1}^{k-2} \binom{k+1}{i} \binom{n - k - 1}{k - 1 - i} + \binom{n - k - 1}{k - 1}.$

Proof. For $k = \frac{n}{2}$, the minimum degree vertices are the k + 1 element subsets and k - 1 element subsets of S_n . As in the Theorem 3.3, the number of 2's in the $M_{\delta}DM(H_T(n,k))$ is

$$\binom{k-1}{k-2}\binom{n-k+1}{1} + \binom{k+1}{k-1} = (k-1)(n-k+1) + (k+1)$$

and the number of 4's are $\binom{n-k+1}{k-1} + \sum_{i=1}^{k-2} \binom{k+1}{i} \binom{n-k-1}{k-1-i} + \binom{n-k-1}{k-1}$. Thus by the Definition 3.1, we have the result.

When n = 4 and k = 2, the minimum degree Wiener index for the graph $H_T(n, k)$ is given as follows:

Result 3.5. The minimum degree Wiener index for the graph $H_T(4,2)$ is 64.

Proof. In minimum δ -distance matrix, each row contains $\binom{k-1}{k-2}(n-k+1) + \binom{k+1}{k-1}$ vertex pairs at a distance 2 and $\binom{n-k-1}{k-1}$ vertex pairs with distance 4. Since $n = 4, k = \frac{n}{2} = 2$, there are 6 and 1 unordered vertex pairs at distance 2 and 4 in each row, respectively. As the order of the minimum δ -distance matrix is $\binom{n}{k-1} + \binom{n}{k+1} = 8, MDW(H_T(n,k)) = 64.$

The minimum δ -distance matrix for various graphs, including molecular graphs from chemistry, exhibits an interesting property that can be found. The sums of the elements in each row of the minimum δ -distance matrices are equal in the case of the bipartite Kneser type-k graphs.

Theorem 3.6. Let G be the bipartite Kneser type-k graph $H_T(n,k), n > 3, 1 \le k \le \lfloor \frac{n}{2} \rfloor$. Let R_i denote the *i*th row of the minimum δ -distance matrix of G. Then the sum $S(R_i) = \sum_{i=1}^{|V_{min}|} U_{ij}$ is the same for each $i = 1, 2, 3, ..., |V_{min}|$.

Proof. In the graph $H_T(n,k)$, the vertices with minimum degree occur only in the partite set V_2 . For any unordered pair of vertices U_1, U_2 in $V_2, d(U_1, U_2)$ is either 2 or 4.

Case 1: When $k \neq \frac{n}{2}$. The number of 2's in the ith row, $i = 1, 2, \ldots, |V_{min}|$, of

the minimum δ -distance matrix is (n-k-1)(k+1) and that of 4 is $\binom{n-k-1}{k+1} + \sum_{l=1}^{k-1} \binom{k+1}{l} \binom{n-k-1}{k+1-l}$. Thus $S(R_i) = \sum_{j=1}^{|V_{min}|} U_{ij}$ $= 2(n-k-1)(k+1) + 4 \left[\binom{n-k-1}{k+1} + \sum_{l=1}^{k-1} \binom{k+1}{l} \binom{n-k-1}{k+1-l} \right].$

Case 2: When $k = \frac{n}{2}$. Using Theorem 3.4, for $i = 1, 2, ..., |V_{min}|, S(R_i) = 2d(G, 2) + 4d(G, 4)$.

Definition 3.7. On the basis of minimum degree Wiener index, let us define minimum degree Wiener polynomial for a simple connected graph G as ${}^{d(G)}_{MDH(G, r)} = \sum_{i=1}^{d} d(G, h) x^{h} + |V_{min}| \text{ where } h = d(U_i, U_i) \quad U_i \mid U_i \in V_{min}$

$$MDH(G, x) = \sum_{h=1}^{n} d(G, h)x^n + |V_{min}|$$
, where $h = d(U_i, U_j)$, $U_i, U_j \in V_{min}$,
 $d(G)$ denotes the diameter of the graph G and $d(G, h)$ denotes the number of

d(G) denotes the diameter of the graph G, and d(G, h) denotes the number of unordered pairs of minimum-degree vertices at a distance h.

Theorem 3.8. The minimum degree Wiener polynomial of the bipartite Kneser type-k graphs $H_T(n,k), n > 1, k \neq \frac{n}{2}$ is given by

$$MDH(H_T(n,k)) = \frac{\binom{n}{k+1}}{2} \left[(n-k-1)(k+1) \right] x^2 + \frac{\binom{n}{k+1}}{2} \left[\binom{n-k-1}{k+1} + \sum_{i=1}^{k-1} \binom{k+1}{i} \binom{n-k-1}{k+1-i} \right] x^4 + \binom{n}{k+1}$$

Proof. The result follows from Theorem 3.3 and Definition 3.7.

Theorem 3.9. The minimum degree Wiener polynomial of the bipartite Kneser type-k graphs $H_T(n,k), n > 1, k = \frac{n}{2}, n \neq 4$ is given by

$$MDH(H_T(n,k)) = \frac{\binom{n}{k-1} + \binom{n}{k+1}}{2} \left[d(G,2) \ x^2 + d(G,4) \ x^4 \right] + \binom{n}{k-1} + \binom{n}{k+1},$$

where d(G,2) and d(G,4) are as in Theorem 3.4.

Proof. Using Theorem 3.4 and Definition 3.7, the result holds.

Corollary 3.10. The minimum degree Wiener polynomial for the graph $H_T(4, 2)$ is $4x^4 + 24x^2 + 8$.

Let us consider some other non regular graphs (only minimum degree vertices are labelled).



The minimum degree Wiener polynomial for the graph G_1 in Figure: 2 is $3x^3 + 3$. The minimum degree Wiener polynomial for a 3-path irregular tree of order 11 (see the graph G_2 in Figure :3) is $2x^2 + 4x^5 + 4x^6 + 5$.

Wiener polarity index. Another topological descriptor, the Wiener polarity index, was developed by Wiener and is known to be connected to the cluster coefficient of networks. The Wiener Polarity index [1] $W_p(G)$ is defined to be the number of unordered pairs of vertices at distance 3 in G. Then we find the Wiener polarity index of $H_T(n, k)$ graphs.

Theorem 3.11. The Wiener polarity index of the graph $H_T(n,k)$ is given by

$$W_p(H_T(n,k)) = \binom{n}{k} \left(2^n - 1 - \binom{n}{k}\right) - \left(2^k + 2^{n-k} - 3\right)\binom{n}{k}.$$

Proof. In the case of $H_T(n, k)$, the distance between any pair (U, W) of vertices is 3 only when $U \in V_1$, $W \in V_2$ and $UW \notin E(H_T(n, k))$. Since the size of the graph is $(2^k + 2^{n-k} - 3)\binom{n}{k}$, the number of unordered pairs of vertices at distance 3 is $\binom{n}{k}(2^n - 1 - \binom{n}{k}) - (2^k + 2^{n-k} - 3)\binom{n}{k}$ and it is the Wiener polarity index. \Box

3.2. Minimum degree Wiener index for Johnson graphs, bipartite Kneser graphs and set inclusion graphs. The Johnson graph J(n, k) is the graph whose vertices are the k element subsets of S_n as well, where two vertices U and W are adjacent if $|U \cap W| = k - 1$. Whereas the bipartite Kneser graph

H(n,k), n > 1 has a vertex set consisting of all k and n - k element subsets of S_n and adjacency exists when one of them is a subset of the other.

As both the Johnson graphs and the bipartite Kneser graphs are regular graphs, the minimum degree Wiener index is the same as the usual Wiener index.

The set inclusion graph $G(n, k^*, l)$ [11], where $1 \le k^* < l \le n-1, k^*+l \le n$ is the graph with vertices as k^* -element and *l*-element subsets of S_n , adjacency exist if one of them contained in another. Its minimum degree is $\delta(G(n, k^*, l)) = min\{\binom{n-k^*}{l-k^*}, \binom{l}{k^*}\}$.

Whenever $k^* + l = n$, the set inclusion graph $G(n, k^*, l)$, becomes regular graph and hence the minimum degree Wiener index and the ordinary Wiener index are the same. The minimum δ -distance matrices of set inclusion graphs such as G(5, 1, 3) and G(6, 1, 4) are symmetric matrices with entries 0 and 2. Hence we have the following theorem:

Theorem 3.12. In the set inclusion graph $G(n, k^*, l)$ with $k^* + l = n$, the minimum degree Wiener index is the same as the Wiener index and if $k^* + l < n$, then the minimum degree Wiener index of $G(n, k^*, l)$ is the same as that of $H_T(n, k)$ for some k.

Proof. If $k^* + l = n$, then the graph $G(n, k^*, l) = G(n, k^*, n - k^*)$ has $2\binom{n}{k^*}$ vertices, with a degree of $\binom{n-k^*}{k^*}$ for each vertex. Hence it is a regular graph. Thus from the Definition 3.1 and the Observation 1, the minimum degree Wiener index of $G(n, k^*, n - k^*)$ is the same as the Wiener index. If $k^* + l < n$, then for some k in $H_T(n, k)$, in particular when k = l - 1, both the graphs $G(n, k^*, l)$ and $H_T(n, k)$ have the same minimum degree Wiener index. \Box

Remark 3.13.

$$MDW(G(4,1,2)) = MDW(H_T(4,1)),$$

$$MDW(G(6,1,2)) = MDW(H_T(6,1)).$$

All additive topological indices of a graph G can be expressed mathematically as $\sum F(x, y)$, where the summation runs over all edges of the graph with degree of end vertices as x and y. The distance-based topological indices are very useful in social networks. In the next section, the distance-based indices like Wiener index and hyper-Wiener index of the graphs $H_T(n, k)$ for $n \ge 4$ and k = 2, 3 are computed.

3.3. Wiener index of $H_T(n, 2)$. Let G be a graph with vertex set V(G). The Wiener index, W(G) is defined as the sum of distances between all unordered pairs of vertices of the graph G. That is, $W(G) = \sum_{U,W \in V(G)} d(U,W)$. Here, we

determined the Wiener index of the graphs $H_T(n, 2)$ and $H_T(n, 3)$.

Theorem 3.14. For $n \ge 4$, the Wiener index of the graph $H_T(n, 2)$ is given by

$$W(H_T(n,2)) = \frac{n^2 - n}{2} \left[5 \times 2^{n-1} - \frac{n^2 - n}{2} - 7 \right] + \frac{(2^{n+1} - n^2 + n - 2)(2^{n+1} - n^2 + n - 4)}{2} - 2D(n,2)$$

where

$$D(n,2) = \begin{cases} \frac{(n^2 - n)(n^2 - n + 2)}{8} + 2^{n-1}(n+2) - \frac{n}{2}(3n+1) - 2\\ + \frac{1}{2}\sum_{j=3}^{n-1} \binom{n}{j} \left[\sum_{r=2}^{j-1} \binom{j}{r}\binom{n-j}{j-r}\right] + \sum_{i=3,n\neq 4}^{n-2} \left\{\sum_{j=i+1}^{n-1} \binom{n}{j} \left[\sum_{p=2}^{i} \binom{j}{p}\binom{n-j}{i-p}\right]\right\}$$
(3.1)

Proof. Consider the graph $H_T(n, 2)$. Using combinatorics and by counting techniques, we get the number of unordered pairs of vertices with distance d, $\mathcal{N}^2_d(U, W)$ as

$$\mathcal{N}_{d}^{2}(U,W) = \begin{cases} \frac{n}{8}(n-1)(2^{n}+4) & \text{if } d = 1, \\ D(n,2) & \text{if } d = 2, \\ \frac{n}{8}\left[3 \times 2^{n}(n-1) - 2n^{2}(n-2) - 2(5n-4)\right] & \text{if } d = 3, \\ \frac{1}{8}\left[(n^{2}-n)(n^{2}-n-2) + (2^{n+1}-n^{2}+n-2)(2^{n+1}-n^{2}+n-4)\right] - D(n,2) & \text{if } d = 4, \end{cases}$$
(3.2)

where D(n, 2) is the Equation 3.1. Thus Wiener index is given by,

$$W(H_T(n,2)) = \sum_{U,W \in V(H_T(n,2))} d(U,W)$$

= $\frac{n}{8}(n-1)(2^n+4) + 2D(n,2) + \frac{3n}{8} [3 \times 2^n(n-1) - 2n^2(n-2) - 2(5n-4)]$
+ $\frac{1}{2} [(n^2-n)(n^2-n-2) + (2^{n+1}-n^2+n-2)(2^{n+1}-n^2+n-4)] - 4D(n,2)$
= $5 \times 2^{n-2}(n^2-n) - 5\frac{n^2-n}{2} - 3\left[\frac{n^2-n}{2}\right]^2 + 4\binom{\binom{n}{2}}{2} + 4\binom{\binom{2n}{2}}{2} - 2D(n,2)$
= $\frac{n^2-n}{2} [5 \times 2^{n-1} - \frac{n^2-n}{2} - 7] + \frac{(2^{n+1}-n^2+n-2)(2^{n+1}-n^2+n-4)}{2} - 2D(n,2).$

Remark 3.15. The Wiener index of the graph $H_T(3,2)$ is 36.

Proof. Using the Definition 2.1, the part V_1 of vertex set of $H_T(3,2)$ contains 3 vertices and V_2 has 4 elements. The diameter of the graph is 3. Also, the number of unordered pairs of vertices with distance 1 is 9, with distance 2 is 9, and with distance 3 is 3. Thus, $W(H_T(3,2)) = 9 + 18 + 9 = 36.$

Now, we are going to find the Wiener index of the graph $H_T(n,3)$ as follows:

Theorem 3.16. The Wiener index of the bipartite Kneser type-3 graph, for $n \ge 4$, is given by

$$W(H_T(n,3)) = \frac{(n^2 - n)(n - 2)}{6} \left[11 \times 2^{n-2} - 13 - 3\binom{n}{3} \right] + 4\binom{\binom{n}{3}}{2} + 4\binom{2^n - 1 - \binom{n}{3}}{2} - 2D(n,3),$$

where

$$D(n,3) = \sum_{j=1,3} \binom{\binom{n}{j}}{2} + \sum_{i=1}^{2} \sum_{j=4}^{n} \binom{n}{j} \binom{j}{i} + \frac{1}{2} \sum_{j=4}^{n-1} \binom{n}{j} \left[\sum_{r=3}^{j-1} \binom{j}{r} \binom{n-j}{j-r} \right] + \sum_{i=4}^{n-2} \left\{ \sum_{j=i+1}^{n-1} \binom{n}{j} \left[\sum_{p=3}^{i} \binom{j}{p} \binom{n-j}{i-p} \right] \right\} + \sum_{i=4}^{n-1} \binom{n}{i} + n(n-1)^{2}.$$
(3.3)

Proof. In the case of $H_T(n,3)$, the number of unordered pairs of vertices with distance d is as follows.

$$\mathcal{N}_{d}^{3}(U,W)) = \begin{cases} \frac{1}{6}(n^{2}-n)(n-2)(5+2^{n-3}) & \text{if } d = 1, \\ D(n,3) & \text{if } d = 2, \\ \frac{(n^{2}-n)(n-2)}{6} \left[7 \times 2^{n-3} - \frac{(n^{2}-n)(n-2)}{6} - 6\right] & \text{if } d = 3, \\ \frac{(n^{2}-n)(n-2)\left[(n^{2}-n)(n-2) - 6\right]}{72} + \binom{2^{n-1}-\binom{n}{3}}{2} - D(n,3) & \text{if } d = 4, \end{cases}$$
(3.4)

where D(n,3) is the Equation 3.3.

$$\begin{split} W(H_T(n,3)) &= \frac{1}{6}(n^2 - n)(n - 2)(5 + 2^{n-3}) + 2D(n,3) \\ &+ \frac{(n^2 - n)(n - 2)}{2} \left[7 \times 2^{n-3} - \frac{(n^2 - n)(n - 2)}{6} - 6 \right] \\ &+ \frac{(n^2 - n)(n - 2)\left[(n^2 - n)(n - 2) - 6\right]}{18} + 4 \binom{2^n - 1 - \binom{n}{3}}{2} - 4D(n,3) \\ &= 22 \times 2^{n-3} \frac{(n^2 - n)(n - 2)}{6} - 13 \frac{(n^2 - n)(n - 2)}{6} - 3 \left[\frac{(n^2 - n)(n - 2)}{6} \right]^2 \\ &+ \frac{(n^2 - n)(n - 2)\left[(n^2 - n)(n - 2) - 6\right]}{18} + 4 \binom{2^n - 1 - \binom{n}{3}}{2} - 2D(n,3) \\ &= \frac{(n^2 - n)(n - 2)}{6} \left[11 \times 2^{n-2} - 13 - 3\binom{n}{3} \right] + 4\binom{\binom{n}{3}}{2} + 4\binom{2^n - 1 - \binom{n}{3}}{2} - 2D(n,3) \\ & \Box \end{split}$$

3.4. Hyper-Wiener index of $H_T(n, 2)$. Milan Randic first introduced the hyper Wiener index in 1993. The hyper-Wiener index of a graph G, $WW(G) = \frac{1}{2} \left[\sum d^2(U, W) + \sum d(U, W) \right]$, was given by Klein, Lukovits and Gutman in 1995 [12]. Here we established formulae to find the hyper Wiener index of the graphs $H_T(n, 2)$ and $H_T(n, 3)$.

Theorem 3.17. The hyper Wiener index of the graph $H_T(n, 2)$, $n \ge 4$ is given by

$$WW(H_T(n,2)) = \frac{n^2 - n}{2} \left[19 \times 2^{n-2} - 11 \right] - 6 \left[\frac{n^2 - n}{2} \right]^2 + 10 \binom{\binom{n}{2}}{2} + 10 \binom{\binom{n}{2}}{2} + 10 \binom{\binom{n}{2}}{2} - 7D(n,2),$$

where D(n,2) represents the Equation 3.1 in Theorem 3.14.

Proof.

$$WW(H_T(n,2)) = \frac{1}{2} \left[\sum d^2(U,W) + \sum d(U,W) \right]$$

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$$= \frac{5}{4} (2^{n-1}) (n^2 - n) - \frac{3}{8} (n^2 - n)^2 + \frac{(n^2 - n)(n^2 - n - 2)}{4} + 2\binom{2^n - 1 - \binom{n}{2}}{2}$$
$$- D(n, 2) + \frac{1}{4} (2^{n-2} + 1)(n^2 - n) + 2D(n, 2) + \frac{9(n^2 - n)}{4} \left(2^n - 1 - \binom{n}{2}\right)$$
$$- \frac{9(n^2 - n)}{4} (2^{n-2} + 1) + 8\binom{\binom{n}{2}}{2} + 8\binom{2^n - 1 - \binom{n}{2}}{2} - 8D(n, 2)$$
$$= \frac{n^2 - n}{2} \left[19 \times 2^{n-2} - 11\right] - 6\left[\frac{n^2 - n}{2}\right]^2 + 10\binom{\binom{n}{2}}{2} + 10\binom{\binom{n}{2}}{2} + 10\binom{2^n - 1 - \binom{n}{2}}{2} - 7D(n, 2)$$

Theorem 3.18. The hyper-Wiener index of the graph $H_T(n,3)$, $n \ge 4$ is given by

$$WW(H_T(n,3)) = \binom{n}{3} \left[43 \times 2^{n-3} - 31 \right] - 6\binom{n}{3}^2 + 10\binom{\binom{n}{3}}{2} + 10\binom{\binom{n}{3}}{2} + 10\binom{2^n - 1 - \binom{n}{3}}{2} - 7D(n,3),$$

where D(n,3) represents the Equation 3.3 in Theorem 3.16.

Proof. Using the definition of hyper-Wiener index , we have

$$WW(H_T(n,3)) = \frac{1}{2} \left[(5+2^{n-3}) \binom{n}{3} \right] + D(n,3) + \frac{3}{2} \times \binom{n}{3} \left[2^n - \binom{n}{3} - 2^{n-3} - 6 \right] \\
+ 2\binom{\binom{n}{3}}{2} + 2\binom{2^n - 1 - \binom{n}{3}}{2} - 2D(n,3) + \frac{1}{2} \left[(5+2^{n-3})\binom{n}{3} \right] \\
+ \frac{9}{2} \binom{n}{3} \left[7 \times 2^{n-3} - \binom{n}{3} - 6 \right] + 8\binom{\binom{n}{3}}{2} + 8\binom{2^n - 1 - \binom{n}{3}}{2} - 8D(n,3) \\
= \binom{n}{3} \left[43 \times 2^{n-3} - 31 \right] - 6\binom{n}{3}^2 + 10\binom{\binom{n}{3}}{2} + 10\binom{2^n - 1 - \binom{n}{3}}{2} - 7D(n,3).$$

3.5. Hosoya-Wiener polynomial. The Hosoya polynomial, which H. Hosoya introduced in 1988, can be used to derive all distance-based graph invariants. If d(G, h) represents the number of pairs of vertices having distance h and d(G) denotes the diameter of a graph G, then the Hosoya polynomial [3] is defined as

$$H(G, x) = \sum_{h=1}^{d(G)} d(G, h) x^h$$

Here we consider the alternative definition

$$H(G, x) = \sum_{h=1}^{d(G)} d(G, h) x^h + |V(G)|,$$

which is mentioned in [20]. The hyper-Wiener index and Hosoya-Wiener polynomial for a graph G is related by the equation

$$WW(G) = H'(G,1) + \frac{1}{2}H''(G,1),$$

where H'(G, 1) is the first derivative of H(G, x) at x = 1 [20], is the Wiener index, and H''(G, 1) is the second derivative of H(G, x) at x = 1.

The Hosoya-Wiener polynomial for the graphs $H_T(n, 2)$ and $H_T(n, 3)$ are illustrated in the following theorem.

Theorem 3.19.

$$H(H_T(n,2),x) = \begin{cases} \frac{n}{8}(n-1)(2^n+4)x + D(n,2)x^2 + \left\{\binom{n}{2}\left[3 \times 2^{n-2} - \frac{n^2 - n}{2} - 2\right]\right\}x^3 \\ + \left\{\frac{(n^2 - n)(n^2 - n - 2)}{4} + \binom{2^n - 1 - \binom{n}{2}}{2} - D(n,2)\right\}x^4 + 2^n - 1 \end{cases}$$

where D(n,2) is the same Equation 3.1 in the Theorem 3.14.

$$H(H_T(n,3),x) = \begin{cases} \frac{1}{6}(n^2 - n)(n - 2)(5 + 2^{n-3})x + D(n,3)x^2 + \left\{\binom{n}{3}\left[7 \times 2^{n-3} - \binom{n}{3} - 6\right]\right\}x^3 \\ + \left\{\binom{\binom{n}{3}}{2} + \binom{\binom{2n-1}{3}-\binom{n}{3}}{2} - D(n,3)\right\}x^4 + 2^n - 1 \end{cases}$$

where D(n,3) is as in the Theorem 3.16.

Proof. The proof follows from the definition of Hosoya-Wiener polynomial, Equations 3.2 and 3.4. $\hfill \Box$

The Hosoya-Wiener polynomials for some of the bipartite Kneser type-k graphs are

- $H(H_T(4,1)) = 3x^4 + 16x^3 + 58x^2 + 28x + 15.$
- $H(H_T(4,2)) = 4x^4 + 24x^3 + 47x^2 + 30x + 15.$
- $H(H_T(5,2)) = 40x^4 + 120x^3 + 215x^2 + 90x + 31.$
- $H(H_T(6,3)) = 291x^4 + 600x^3 + 802x^2 + 260x + 63.$

Hence the hyper-Wiener index can be calculated for these graphs from the corresponding first and second derivative of these polynomials.

4. Conclusion

In this paper, Minimum degree Wiener index and minimum degree Wiener polynomial are introduced for any simple connected graph G and computed the same for $H_T(n, k)$, and compared the results with that of bipartite Kneser graphs, Johnson graphs and the set inclusion graphs. Also, we determined the formula for the Wiener index, hyper Wiener index, Wiener polarity index and Hosoya-Wiener polynomial for the bipartite Kneser type-k graphs for k = 2, 3. We introduced minimum δ - distance matrix for a connected graph. The row sums of minimum δ - distance matrix are equal for the graph $H_T(n, k)$. In most of the matrices defined for a graph, this is not so.

Conflicts of interest : The authors hereby declare that there is no potential conflict of interest.

References

- 1. M. Adnan, S.A.U.H. Bokhary and M. Imran, On Wiener polarity index and Wiener index of certain triangular networks, Journal of Chemistry (2021), 1-20.
- J. Bamberg, A. Devillers, M. Ioppolo and C.E. Praeger, Codes and designs in Johnson graphs from symplectic actions on quadratic forms, 2022. ArXiv preprint, arXiv:2202.06237
- G. Cash, S. Klavžar and M. Petkovšek, Three methods for calculation of the hyper-Wiener index of molecular graphs, Journal of Chemical Information and Computer Sciences 42 (2002), 571-576, PMID: 12086516.
- T. Chowdhury and A. Pramanik, *LDPC code construction from bipartite Kneser graphs*, Proceedings of the 2nd International Conference on Communication, Devices and Computing, Springer, 2020, 1-12.
- A.A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, Acta Applicandae Mathematicae 66 (2001), 211–249.
- 6. I. Gutman, Degree-based topological indices, Croatica Chemica Acta 86 (2013), 351-361.
- I. Gutman and B. Furtula, A survey on terminal Wiener index, Novel Molecular Structure Descriptors-Theory and Applications I, Univ. Kragujevac, Kragujevac 173 (2010), 173-190.
- I. Gutman, B. Furtula and M. Petrović, *Terminal Wiener index*, Journal of Mathematical Chemistry 46 (2009), 522-531.
- 9. B. Horvat, T. Pisanski and M. Randic, *Terminal polynomials and star-like graphs*, MATCH Communications in Mathematical and in Computer Chemistry **60** (2008), 493-512.
- H. Hua, On the peripheral Wiener index of graphs, Discrete Applied Mathematics 258 (2019), 135-142.
- 11. X. Huang, Q. Huang and J. Wang, The spectrum and automorphism group of the setinclusion graph, Algebra Colloquium 28 (2021), 497-506.
- D.J. Klein, I. Lukovits and I. Gutman, On the definition of the hyper-Wiener index for cycle-containing structures, Journal of Chemical Information and Computer Sciences 35 (1995), 50-52.
- S.M. Mirafzal, The automorphism group of the bipartite Kneser graph, Proceedings-Mathematical Sciences 129 (2019), 1-8.
- M. Randic, J. Zupan and D. Vikić-Topić, On representations of proteins by star-like graph, Journal of Molecular Graphics and Modelling 26 (2007), 290-305.
- A. Saleh, S. Bazhear and N. Muthana, Uphill Zagreb indices of some graph operations for certain graphs, J. Appl. Math. and Informatics 40 (2022), 959-977.
- S.V. Siva Rama Raju., On a variant of vertex edge domination, J. Appl. Math. and Informatics 41.4 (2023): 741-752
- 17. P. Sreeja, K.G. Sreekumar and K. Manilal, On the diameter and connectivity of bipartite Kneser type-k graphs, Journal of Algebraic Systems (in press).
- 18. K.G. Sreekumar and K. Manilal, Automorphism groups of some families of bipartite graphs, Electronic Journal of Graph Theory and Applications 9 (2021), 65-75.
- K.G. Sreekumar, P. Ramesh Kumar and K. Manilal, Automorphism groups of bipartite Kneser type-k graphs, Asian-European Journal of Mathematics 16 (2023), 2350047.
- B. Zmazek and J. Zerovnik, On generalization of the Hosoya-Wiener polynomial, MATCH Communications in Mathematical and in Computer Chemistry 55 (2006), 359-362.

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