Wiener Index of Some Cycle Related Graphs using Matlab

K. Thilakam
Seethalakshmi Ramaswami College,
Tiruchirappalli – 620 002, Tamil Nadu, India

A. Sumathi
Seethalakshmi Ramaswami College,
Tiruchirappalli – 620 002, Tamil Nadu, India

ABSTRACT
The Wiener index is one of the oldest molecular-graph-based structure-descriptors. It was first proposed by American Chemist Harold Wiener in 1947 as an aid to determine the boiling point of paraffin. The study of Wiener index is one of the current areas of research in mathematical chemistry. It also gives good correlations between Wiener index (of molecular graphs) and the physico-chemical properties of the underlying organic compounds. That is, the Wiener index of a molecular graph provides a rough measure of the compactness of the underlying molecule. The Wiener index W(G) of a connected graph G is the sum of the distances between all pairs (ordered) of vertices of G. $W(G) = \frac{1}{2}\sum_{u,v} d(u,v)$

In this paper, we give the program for calculating the Wiener index of Cata-condensed Cyclic graph and two cycles sharing their edges using MATLAB and discuss the coincidence of Wiener indices of Cata-condensed Cyclic graph with its characteristic graph and give the Wiener number for two Cycles sharing maximum and minimum number of edges.

Keywords
Cycle, Distance, Wiener index, MATLAB

1. INTRODUCTION
Wiener index is a well-known graph distance invariant introduced by Harold Wiener 50 years ago[11]. It is defined as the half sum of the distances between all pairs of vertices of G.

$$W(G) = \frac{1}{2}\sum_{u,v} d(u,v)$$

Where d(u,v) is the number of edges in a shortest path connecting the vertices u & v in G.

Notation:

$$W(G) = \frac{1}{2}\sum_{u,v} d(u,v) = \sum_{u<v} d(u,v) = \sum_{u_i<v_j} d(u_i, v_j)$$

In this paper, we consider finite, nontrivial, simple and undirected graphs. For a graph G, we denote by V(G) and E(G), its vertex and edge sets, respectively[3],[4]. A topological index of a graph G is a numeric quantity related to G. The adjacency matrix of a molecular graph G with n vertices is an n×n matrix.

A = { a_{ij} } defined by:
a_{ij}= 1, if vertices i and j are connected by an edge
0, otherwise.

In the following section, a MATLAB program is presented which is useful for computing the Wiener index some cycle related graphs. We apply this program to compute the adjacency and distance matrices, Wiener indices of the molecular graph.

2. A MATLAB PROGRAM FOR COMPUTING THE WIENER INDEX OF A CATA-CONDENSED CYCLIC GRAPH
In [1],[2] Andrey A. Dobrynin has demonstrated about the W-values of Cata-condensed Benzenoid graph and hexagonal Chains. In a similar way, Now we define a class of graphs which include molecular graph of Cata-condensed cyclic hydro carbons. These Cyclic graphs are composed exclusively of m, n membered Cycles.The Characteristic graph of a given Cyclic graph consists of vertices corresponding to cycle of a graph; two vertices are adjacent iff the corresponding Cycle share an edge. The Cyclic graph is called Cata-condensed if its Characteristic graph is a tree. Here the Characteristic graph of the above graph is isomorphic to star tree. An example of a Cata-condensed Cyclic graph and its Characteristic graph is shown in fig.1b. In other words it is called a special case of super subdivision of C_m. Therefore these Cata-condensed Cyclic graph H of G is denoted by SS(C_m,C_n).**Subdivision** of a graph S(G) is the graph obtained from *G* by replacing each of its edge by a path of length two, or equivalently, by inserting an additional vertex into each edge of *G* . Sethuraman. G and Selvaraju .P have introduced an interesting method of construction of super subdivision of graphs [6]. They defined as, a graph H is said to be **arbitrary super subdivision** of G if H is obtained from G by replacing every edge e_i of G by a complete bipartite graph K_{2,m_i} for some m_i ,1 ≤ i ≤ t, (m_i may vary for each edge e_i) in such a way that the ends of e_i are merged with the two vertices of the 2-vertices part of K_{2,m_i}, after removing the edge e_i from G. It is denoted by **SS(G)** .Recently N. Sridharan and K. Thilakam have determined the Wiener number of super subdivisions of $P_n, C_n, K_{1,n}$ [7]. K. Thilakam & A. Sumathi also have determined Wiener Number of Arbitrary Super Subdivisions of Wheel W_n and Fan F_n [8] and Wiener Index of Arbitrary super subdivision of some cycle related graphs [9]. A graph H is said to be **a super subdivision of a Cycle with Cycle** if H is obtained from the Cycle C_m by replacing every edge e of C_m by C_n. It is denoted by **SS(C_m;C_n)** .It is shown in fig. 1a

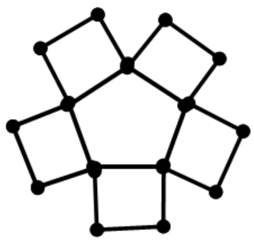


Fig. 1a

SS(C$_5$;C$_4$)

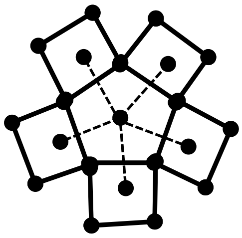


Fig. 1b

SS(C$_5$;C$_4$) with characteristic graph

Here, cycles of a cata-condensed cyclic graph are angularly connected. Each angularly connected cycle is said to correspond to kink in the graph. We now derive new necessary and sufficient conditions that provide the rule of modulo m and m/2 for Wiener indices of cata-condensed cyclic graph and its characteristic graph.

Theorem: 2.1

Let G be a Cycle graph with m vertices and H be the Cata-condensed cyclic graph of G. H' be the characteristic graph of H then

$$W(H) \equiv W(H') \bmod (m) \quad \text{if } m \text{ be odd}$$
$$W(H) \equiv W(H') \bmod (m/2) \quad \text{if } m \text{ be even}$$

Proof

Case1: When m be odd

Since $W(H') \equiv W(K_{1,m}) \equiv 0 \bmod (m)$
and $W(H) \equiv 0 \bmod (m)$

Therefore

$$W(H) \equiv W(H') \bmod (m)$$

Case2: When m be even

Since $W(H') \equiv W(K_{1,m}) \equiv 0 \bmod (m/2)$
and $W(H) \equiv 0 \bmod (m/2)$

Therefore

$$W(H) \equiv W(H') \bmod (m/2)$$

As a continuation of the work in [10] , We compute the Wiener indices of SS(C_m;C_n) for all m,n≥3

Programme: 2.1.1

```
m= input('Cycle with vertices m=');
n= input('Cycle with vertices n=');
A=[];
for i=1:m*(n-1)
    for i=1:(m*(n-1))-1
      A(i,i+1)=1;A(i+1,i)=1;
      for i = m*(n-1)
      A(1,i)=1;A(i,1)=1;
      end
    end
end
 for i=1:n-1:(m*(n-1))-(2*n)+4
       A(i,i+n-1)=1;A(i+n-1,i)=1;
        A(1,(m*(n-1))-n+2)=1;A((m*(n-1))-n+2,1)=1;
end
A;
G = sparse(A);
disp('Distance matrix')
DM = graphallshortestpaths(G,'directed',false)
M=sum(sum(DM));
fprintf('Wiener index of sup.sub.of Cm with Cn, W = %d \n', M/2)
```

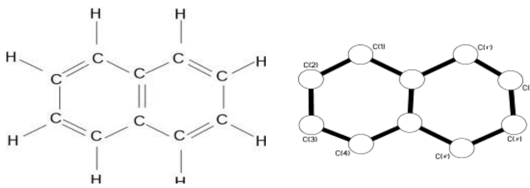
Table 1: Values of W(SS(C_m;C_n)), for 3 ≤ n ≤ 10.

Wiener Indices		**n**							
		3	**4**	**5**	**6**	**7**	**8**	**9**	**10**
m	**3**	**21**	**69**	**153**	**291**	**486**	**759**	**1110**	**1563**
	4	**46**	**152**	**318**	**608**	**986**	**1544**	**2218**	**3128**
	5	**85**	**265**	**555**	**1035**	**1680**	**2595**	**3730**	**5215**
	6	**141**	**435**	**885**	**1647**	**2631**	**4059**	**5775**	**8067**
	7	**217**	**644**	**1309**	**2394**	**3822**	**5838**	**8302**	**11522**
	8	**316**	**928**	**1852**	**3376**	**5332**	**8128**	**11476**	**15904**
	9	**441**	**1260**	**2511**	**4518**	**7128**	**10782**	**15210**	**20970**
	10	**595**	**1685**	**3315**	**5945**	**9305**	**14045**	**19705**	**27125**

3. A MATLAB PROGRAM FOR COMPUTING THE WIENER INDEX OF TWO CYCLES SHARING THEIR EDGES

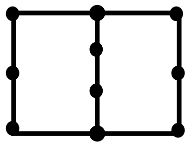
Definition: 3.1

Take two copies of cycle with n vertices then maximum possibility of sharing edges be n-2. If it shares n edges, then the resultant graph be cycle with n vertices. If it shares n-1 edges, then multiple edges arises. Suppose it shares 1, 2,……n-2 edges then finding Wiener indices are very difficult.



NAPHTHALENE **C_6 sharing 1 edge with C_6**

Fig.2a



C_7 sharing 3 edges with C_7

Fig.2b

Theorem:3.1

Wiener index of two cycles with n vertices sharing t edges is

$$W(S(C_n;t)) = \frac{1}{8}\left[n^3 + 2n^2 - n + 14\right] \text{ when n is odd },\; n \geq 5 \;\; t = n-2$$

$$\frac{1}{8}\left[n^3 + 2n^2 + 16\right] \text{ when n is even},\; t=n-2$$

$$W(S(C_n;t)) = \frac{1}{4}\left[3n^3 + 42n^2 + 285n - 530\right] \text{ when n is odd },\; t = 1$$

$$\frac{1}{4}\left[3n^3 - 6n^2 + 4\right] \text{ when n is even, t=1}$$

$$W(S(C_n;t)) = \begin{cases} \frac{1}{8}n^3 & \text{when n even, t=n} \\ \frac{1}{8}(n-1)n(n+1) & \text{when n odd, t=n} \end{cases}$$

The following Programme illustrates Wiener index of two cycles with n vertices sharing t edges

Programme:3.2.1

```
n= input('Cycle with vertices n=');
t= input(' No. of edges sharing =');
A=[];
 if t<=n-3
 for i=1:n
      for i=1:n-1
       A(i,i+1)=1;A(i+1,i)=1;
       for i = n
       A(1,i)=1;A(i,1)=1;
       end
      end
 end
 for i=n+1:(2*n)-t-2
       A(i,i+1)=1;A(i+1,i)=1;
       A(1,n+1)=1;A(n+1,1)=1;
       A(t+1,(2*n)-t-1)=1;A((2*n)-t-1,t+1)=1;
 end
 elseif t==n-2
      for i=1:n
      for i=1:n-1
       A(i,i+1)=1;A(i+1,i)=1;
       for i = n
       A(1,i)=1;A(i,1)=1;
       end
       end
 end
       A(1,n+1)=1;A(n+1,1)=1;
       A(t+1,(2*n)-t-1)=1;A((2*n)-t-1,t+1)=1;
 end
 if t==n-1
          disp('Parallel edges arises')
          disp('Cannot be determined')
 elseif t==n
          disp('Both cycles are identified')
          disp('Cycle with n vertices')
 end
A;
G = sparse(A);
disp('Distance matrix')
DM = graphallshortestpaths(G,'directed',false)
M=sum(sum(DM));
fprintf('Wiener index of G sharing t edges, W = %d \n' , M/2)
```

Table 2: Values of $W(S(C_n;t))$, for $3 \le n \le 10$.

Wiener Indices		t							
		1	2	3	4	5	6	7	8
n	3	7	-						
	4	25	14	-					
	5	55	36	23	-				
	6	109	78	54	38	-			
	7	181	138	102	75	56	-		
	8	289	230	178	136	105	82	-	
	9	421	346	278	220	174	139	112	-
	10	601	506	418	340	275	224	184	152

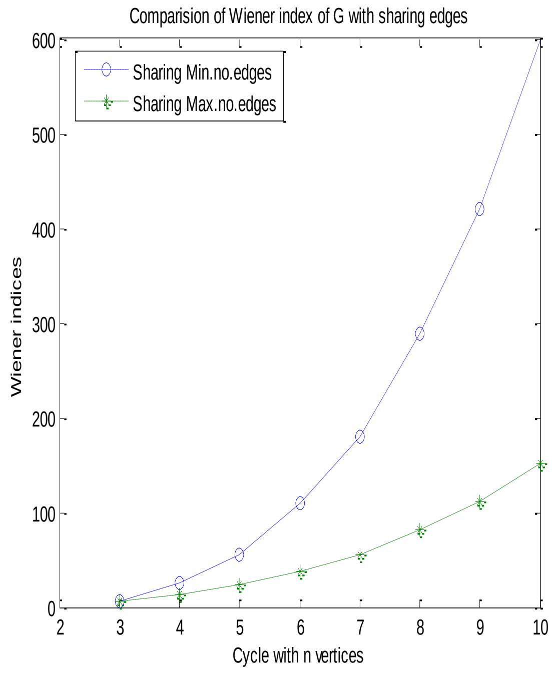


Fig. 3

4. CONCLUSION

In this paper, we have given Wiener indices for the special type of super sub division of cycle graph and discussed the congruence relation between W(H) its characteristic graph. In section 3, we have compared Wiener indices of two equally membered cycles shares maximum and minimum edges. Fig. 3 illustrates that $W(S(C_n;t))$ is maximum if it shares minimum number of edges and it is minimum if it shares maximum number of edges. If two cycles shares all the edges together then $W(S(C_n;t))= W(C_n)$

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