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Wiener Index and Maximum Eccentricity Energy for A Cycle Graph

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ABSTRACT

In this paper, we study the concepts of Wiener Index of Cycle graph & its Maximum Eccentricity Energy, EM_e (C). The Maximum Eccentricity Energy for Cycle is derived with examples and Application of Wiener Index in chemistry is also discussed.

Keywords : Wiener Index, Cycle, Maximum Eccentricity Energy.

I. INTRODUCTION

A graph G = (V,E) is a simple graph, that is, having loops, no multiple and directed edges. In graph theory, a Cycle graph or circular graph is a graph that consists of a single Cycle, or in other words, some number of vertices connected in a closed chain. The Cycle graph with n vertices is called C_n. The number of vertices in $C_n$equals the number of edges, and every vertex has degree 2; that is, every vertex has exactly two edges incident with it.

II. DEFINITION

2.1 WIENER INDEX:[1]

The Wiener index is named after Harry Wiener who introduced in 1947, at the time, wiener called it the path number. Based on its success, many other topological indexes of chemical graphs based on information in the distance matrix of the graph have been developed subsequently to Wiener's work. The study of Wiener index is one of the current area of research in mathematical chemistry. 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 acid to determining the boiling point of paraffin.

The Wiener index W(G) of a connected graph G is the sum of the distance between all pairs of vertices of G.

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

(or)

$$= \sum_{u<v} d(u,v)$$

Where, $d(u,v)$ is the distance between all pairs of vertices of G.

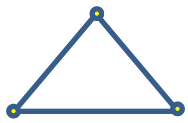
2.2 WIENER INDEX OF A CYCLE:

The Cycle graph with n vertices is denoted by C_n. The number of vertices in $C_n$equals the number of edges, and every vertex has degree 2; that is, every vertex has exactly two edges incident with it.

The Wiener index of a Cycle is calculated using the general formula ,

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

Example:1 when n is odd , n=3

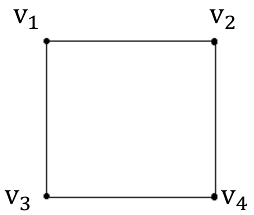


$W(C_n) = \frac{1}{8}(n-1)n(n+1) = \frac{1}{8}(3-1)3(3+1)$

$= \frac{1}{8}*2*3*4$

$W(C_n) = 3.$

Example:2 When n is even ,n=4



$W(C_n) = \frac{1}{8}n^3$

$= \frac{1}{8}(4^3)$

$W(C_n) = 8$

III. THE MAXIMUM ECCENTRICITY ENERGY OF CYCLE GRAPHS:[2]

The distance d(u,v) between any two vertices u and v in a graph G is the length of a minimum path connecting them. For a vertex v of G, The eccentricity of a vertex v is e(v)=max{d(u,v):u∈V(G)}.The radius of G is r(G)= min{e(v):v∈V(G)}.The diameter of G is D(G)= max{e(v):v∈V(G)}.

Let G(V,E) be a simple connected graph with n vertices $v_1, v_2, \ldots, v_n$ *and* e(v_i),be the eccentricity of a vertex v_i, i=1,2,…n.

The Maximum Eccentricity matrix of G defining as, where

$$e_{ij} = \begin{cases} \max\{e(v_i), e(v_j), & If\ v_iv_j \epsilon\ E(G); \\ 0, & otherwise. \end{cases}$$

The characteristic polynomial of the Maximum Eccentricity matrix $M_e(G)$ is defined by

P(G,**λ**)=det(**λ**I-$M_e(G)$)

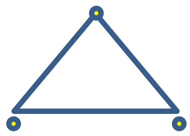
Where I is the unit matrix of order n. The Maximum Eccentricity eigenvalues of G are the eigenvalues of $M_e(G)$. Since $M_e(G)$ is real and symmetric with zero trace, then its eigenvalues the real numbers with sum equals to zero. We label them in non-increasing order $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

The Maximum Eccentricity energy of Cycle graph G is defined as

$$EM_e(G) = \sum_{i=1}^{n} |\lambda_i|.$$

To illustrate this concept, we study the following examples.

Example 3.1



G_1

The Maximum Eccentricity matrix of G_1 is

$$M_e(G_1) = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

The Characteristic polynomial of $M_e(G_1)$ is

P(G_1,**λ**)=det(**λ**I-$M_e(G)$)

$$= \begin{pmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 1 \\ 1 & 1 & -\lambda \end{pmatrix}$$

$= -\lambda^3 + 3\lambda + 2$

The Eigenvalues of G_1 are

$\lambda_1 = 1 \quad \lambda_2 = -1 \quad \lambda_3 = 2$

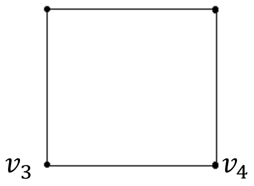
Therefore the Maximum Eccentricity energy of G_1 is

$$EM_e(G) = \sum_{i=1}^{n} |\lambda_i|.$$

$EM_e(G_1) = 4$

***Example* 3.2**

v_1 v_2



G_2

The Maximum Eccentricity matrix of G_2 is

$$M_e(G_2)=\begin{pmatrix} 0 & 2 & 2 & 0 \\ 2 & 0 & 0 & 2 \\ 2 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 \end{pmatrix}$$

The Characteristic polynomial of $M_e(G_2)$ is

$$P(G_2, \boldsymbol{\lambda})=\det(\boldsymbol{\lambda}I-M_e(G))$$

$$=\begin{pmatrix} -\lambda & 2 & 2 & 0 \\ 2 & -\lambda & 0 & 2 \\ 2 & 0 & -\lambda & 2 \\ 0 & 2 & 2 & -\lambda \end{pmatrix}$$

$$= \lambda^4-16\lambda^2$$

$$=\lambda^2(\lambda^2-16)$$

The Eigenvalues of G_2 are

$$\lambda_1 = 0,\ \lambda_2 = 0,\ \lambda_3= -4,\ \lambda_4=4$$

Therefore the Maximum Eccentricity Energy of G_2 is

$$EM_e(G) =\sum_{i=1}^{n} |\lambda_i|.$$

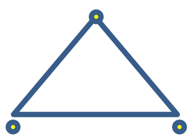
$$EM_e(G_2)=8.$$

Result:[2]

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the Maximum Eccentricity eigenvalues of a Cycle graph G. Then if G=C_n, then

$$\sum_{i=1}^{n} \lambda_i^2 = \begin{cases} n(n-1), & if\ n\ is\ odd; \\ n^2, & if\ n\ is\ even. \end{cases}$$

This can be verified in example



$$M_e(G_1)=\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

The Eigenvalues of G_1 are

$$\lambda_1 = 1 \qquad \lambda_2 = -1 \qquad \lambda_3=2$$

$$\sum_{i=1}^{n} \lambda_i^2 = 1+1+4=6.$$

Result:[2]

Let C_n be the cycle graph with n≥3 vertices. Then the Maximum Eccentricity energy of C_n is

$$EM_e(C_n) = \begin{cases} (n-1)\csc\frac{\pi}{2n}, & if\ n \equiv 1(mod\ )2; \\ 2n\csc\frac{\pi}{2n}, & if\ n \equiv 2(mod\ )4; \\ 2n\cot\frac{\pi}{2n}, & if\ n \equiv 0(mod\ )4; \end{cases}$$

4 Application of wiener index in chemical graph theory:[4]

In organic chemistry, an alkane, or paraffin, is an acyclic saturated hydrocarbon. In other words, an alkane consists of hydrogen and carbon atoms arranged in a tree structure in which all the carbon-carbon bonds are single. Alkanes have the general chemical formula$\boldsymbol{C_nH_{2n+2}}$.

The first application of the Wiener number was for predicting the boiling points **b.p**=$\boldsymbol{\alpha W + \beta w(3) + \gamma}$.

Where α, β, γ are empirical constants, and w(3) is called path number.

i.e) the number of pairs of vertices whose distance is equal to 3.

Wiener Index can also used to estimate boiling points, molar volumeserization. It is used to predict the melting point and other physical properties of polymers, on the basis of their W values. Distance properties of molecular graphs from an important topic in chemical graph theory. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The Wiener index of a graph G is defined as the sum of all distances between distinct vertices of G.Graph theory has found considerable use in chemistry, particularly in modelings chemical structures.

IV. CONCLUSION

In this paper we have derived Wiener Index and Maximum Eccentricity Energy for Cycles. By using this paper, generalized formula for Maximum Eccentricity Energy for Cycles can also be derived by future researchers.

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