ISSN (Online): 2456-5717

International Journal of Advanced Research in Basic Engineering Sciences and Technology (IJARBEST)
Vol.3 Issue.12 December 2017

On the Detour Index of Circular Ladder

S. Prabhu[1], J. Praveen[2]
Assistant Professor, Department of Applied Mathematics, Sri Venkateswara College of Engineering, Sriperumbudur, India [1]
UG Scholar, Department of Chemical Engineering, Sri Venkateswara College of Engineering, Sriperumbudur, India [2]

Abstract— **A topological index is a numeric quantity of a molecule that is mathematically derived from the structural graph of a molecule. The detour index of a connected graph is defined as the sum of the detour distances (lengths of longest paths) between unordered pairs of vertices of the graph. In this paper we find an exact expression for detour index of circular ladder.**

Index Terms— **Detour index, Detour matrix, Molecular Descriptor, Topological index.**

I. Introduction

The structure of a chemical composite can be symbolized by a graph whose vertex and edge identify the atom and bonds respectively. Computational drug design is a rapidly growing field which is now a very important component in the discipline of medicinal chemistry. International Union of Pure and Applied Chemistry (IUPAC), Medicinal Chemistry Section Committee has pointed out the topological index as one among the terms used in computational drug design for easy reference purposes. Topological index is the numeric quantity of molecule that is mathematically derived from the structural graph of a molecule. The topological indices are used in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) studies.

The concept of topological index came from work done by Harold Wiener in 1947 while he was working on boiling point of paraffin [1]. The first topological index in the name of Harold Wiener is the Wiener index is the first topological index established in the field of computational chemistry. The Wiener index of the graph G is defined as [2]

$$W(G) = \sum_{\{u,v\}\subset V(G)} d(u,v)$$

For more details on Wiener index consult [3,4,5]. The detour distance (length of longest path between them) between vertices u and v in G is denoted by $l(u,v)$. Note that $l(u,u) = 0$ for any $u \in V(G)$. The detour index of the graph G is defined as [6,7,8,9]

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$$\omega(G) = \sum_{\{u,v\}\subset V(G)} l(u,v)$$

The detour matrix, together with the distance matrix, was introduced into the mathematical literature in 1969 by Frank Harary [10]. Both matrices were also briefly discussed in 1990 by Buckley and Harary in their book on the concept of distance in graph theory [11]. The detour matrix was introduced into the chemical literature in 1994 under the name the maximum path matrix of a molecular graph by Ivanciuc and Balaban [6] and independently by us in 1995 [7].

The detour matrix can be used to compute the so-called detour index [8] in the same way as the distance matrix [12,13] can be employed to generate the Wiener index [2,14]. The detour index was also introduced by Ivanciuc and Balaban [6] as the sum of the maximum distances between every pair of vertices and independently by John [15]. Lukovits, who introduced the term the detour index, is also very active in studying the properties of this index and its uses in structure-property studies. He reported some of his results on the detour matrix and detour index in this journal and elsewhere [8,16,17]. Lukovits was also first to use this index in structure-property modelling [8]. It has been proved in [11], that the problem of finding the detour matrix is *NP*-complete. A method for constructing the detour matrix for graphs of moderate sizes were presented in [18].

The detour index is equivalent with the Wiener index $W(G)$ in acyclic structures, where only one path exists between every pair of atoms.

II. Preliminaries

Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices u and v in G is the length (number of edges) of a shortest path between them, denoted by $d(u, v)$. Prof. E. Sampath Kumar [19] introduces the detour graph of a given graph G, denoted by $D(G)$ is an edge labeled complete graph in 'n' vertices where $n=|V(G)|$, for every $u,v \in V(G)$ the label for the edge uv is $l(u,v)$. If a detour graph of G has all the labels 1, then $G = K_2$. If a detour graph of G has all the labels 2, then $G = K_3$. The maximum distinct integers one can get in a detour distance sequence is n-1. The graph G is a tree if and only if the detour graph $D(G)$ contains (n-1) 1's. A Graph G is path if and only if the detour distance sequence is $1^{n-1}, 2^{n-2}, \ldots, (n-1)^1$. A graph G is a star if and only if the detour distance sequence of G is

ISSN (Online): 2456-5717

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$1^{n-1}, 2^{\frac{1}{2}(n^2-3n+2)}$. It has been proved that the detour distance sequence for wheel is $n^{\frac{n^2+n}{2}}$. The detour index is the sum of all element in the detour distance sequence.

III. Main Results

Definition 4.1:

Let $a_1, a_2, a_3, \ldots a_n$ and $b_1, b_2, b_3, \ldots b_n$ be two paths of length n. The graph L_n obtained by adding edges $a_i b_i$ where $1 \le i \le n$ is called a *ladder*.

The Ladder with n vertices denoted by L_n has $2n$ vertices and $3n-2$ edges.

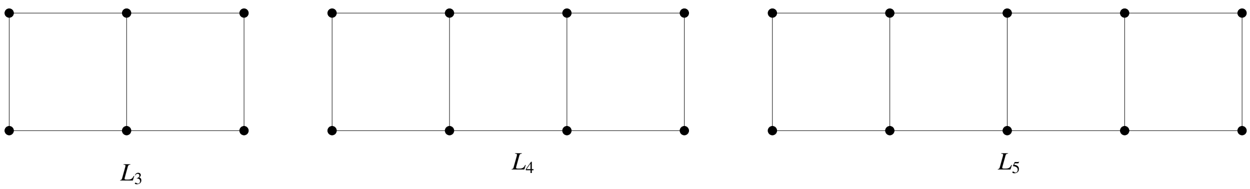

Fig. 1. Ladder of dimension 3,4 and 5

Definition 4.2:

Let $a_1, a_2, a_3, \ldots a_n, a_1$ and $b_1, b_2, b_3, \ldots b_n, b_1$ be two cycles of length. The graph $CL(n)$ obtained by adding edges $a_i b_i$ where $1 \le i \le n$ is called a *circular ladder*. See Figure 1.

The Circular Ladder is also called a *Prism* graph. It has $2n$ vertices and $3n$ edges.

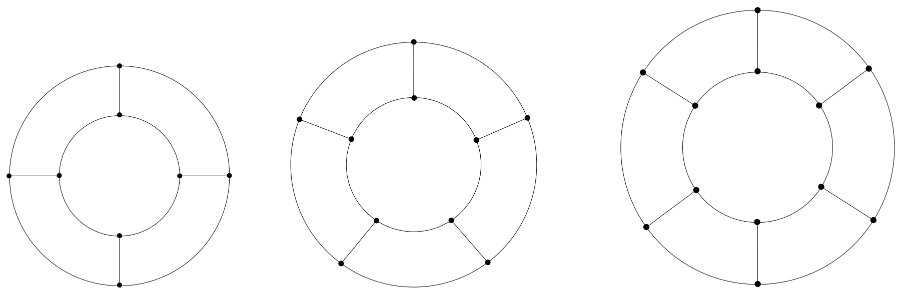

Fig. 2. Circular ladder of dimension 4, 5 and 6

Theorem 1:

Let $G = CL_n$, $n \ge 3$ be a circular ladder. Then $\omega(G) = 4n^3 - 4n^2 + n$, where n is odd.

Proof:

$|V(CL_n)| = 2n$ vertices. Let us claim that the Detour distance between any two vertices of -

-circular ladder CL_n is $2n-1$. Divide CL_n into 2 cycles of n vertices namely inner cycle *IC* and outer cycle *OC*. Let $V(IC)=\{v_1, v_2, v_3, ..., v_n\}$ and $V(OC)=\{u_1, u_2, u_3, ..., u_n\}$.

Case 1:

$x \& y \in V(IC)$.

Case 1.1:

Let $x \& y$ are adjacent. In inner cycle (v_i, v_{i+1}) are adjacent where $1 \le i \le n$ and also there exist a path $v_i, u_i, u_{i+1}, u_{i+2}, \ldots, u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, \ldots, v_{n+i-(n-2)}, v_{n+i-(n-1)}$ of length $2n-1$. This path has v_i as initial and v_{i+1} as terminal vertices of a path.

Case 1.2:

Let $x \& y$ are non-adjacent.

Case 1.2.a(1):

Let the non-adjacent vertices be v_i and v_{i+j} where $j=2$. Then the path of length $2n-1$ is $v_i, u_i, u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, u_{n+i-2}, u_{n+i-3}, v_{n+i-3}, \ldots, u_{n+i-(n-3)}, u_{n+i-(n-2)}, u_{n+i-(n-1)}, v_{n+i-(n-1)}, v_{n+i-(n-2)}$. This path has v_i and v_{i+2} as initial and terminal vertices.

Case1.2.a(2):

Let the non-adjacent vertices be v_i and v_{i+j} where $j=4$.

The required path is $v_i, u_i, u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, u_{n+i-2}, u_{n+i-3}, v_{n+i-3}, \ldots, u_{n+i-(n-5)}, u_{n+i-(n-4)}, u_{n+i-(n-3)}, u_{n+i-(n-2)}, u_{n+i-(n-1)}, v_{n+i-(n-1)}, v_{n+i-(n-2)}, v_{n+i-(n-3)}, v_{n+i-(n-4)}$. This path has v_i and v_{i+4} as initial and terminal vertices.

Case1.2.a(3):

Let the non-adjacent vertices be v_i and v_{i+j} where $j=6$. The path is $v_i, u_i, u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, u_{n+i-2}, u_{n+i-3}, v_{n+i-3}, \ldots, u_{n+i-(n-7)}, u_{n+i-(n-6)}, u_{n+i-(n-5)}, u_{n+i-(n-4)}, u_{n+i-(n-3)}, u_{n+i-(n-2)}, u_{n+i-(n-1)}, v_{n+i-(n-1)}, v_{n+i-(n-2)}, v_{n+i-(n-3)}, v_{n+i-(n-4)}, v_{n+i-(n-5)}, v_{n+i-(n-6)}$). This path has v_i and v_{i+6} as initial and terminal vertices.

Case 1.2.b(1):

Let the non-adjacent vertices be v_i and v_{i+j} where $j=3$. The path is $v_i, u_i, u_{i+1}, v_{i+1}, v_{i+2}, u_{i+2}, u_{i+3}, u_{i+4}, \ldots, u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, v_{n+i-3}, \ldots, v_{n+i-(n-3)}$. This path has v_i and v_{i+3} as initial and terminal vertices.

Case 1.2.b(2):

Let the non-adjacent vertices be v_i and v_{i+j} where $j = 5$. The path is v_i, u_i, u_{i+1}, v_{i+1}, v_{i+2}, u_{i+2}, u_{i+3}, v_{i+3}, v_{i+4}, u_{i+4}, u_{i+5}, u_{i+6}, …., u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, v_{n+i-3}, …., $v_{n+i-(n-5)}$. This path has v_i and v_{i+5} as initial and terminal vertices.

Case 1.2.b(3):

Let the non-adjacent vertices be v_i and v_{i+j} where $j = 7$. The path is v_i, u_i, u_{i+1}, v_{i+1}, v_{i+2}, u_{i+2}, u_{i+3}, v_{i+3}, v_{i+4}, u_{i+4},u_{i+5}, v_{i+5}, v_{i+6}, u_{i+6}, u_{i+7}, u_{i+8}, u_{i+9}, …., u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, v_{n+i-3}, …., $v_{n+i-(n-7)}$. This path has v_i and v_{i+7} as initial and terminal vertices.

Case 2:

Let $x \,\&\, y \in V(OC)$

This case is similar to case 1.

Case 3:

$x \in V(IC) \,\&\, y \in V(OC)$

Case 3.1:

Let $x \,\&\, y$ are adjacent.

Then the path is v_i, v_{n+i-1}, v_{n+i-2}, v_{n+i-3} … $v_{n+i-(n-1)}$, $u_{n+i-(n-1)}$, u_{i+2}, u_{i+3} … u_{i+n}

Case 3.2:

Let $x \,\&\, y$ are non-adjacent.

Then the path is v_i, u_i, u_{n+i-1}, v_{n+i-1}, v_{n+i-2}, u_{n+i-2}, u_{n+i-3}, v_{n+i-3}, v_{n+i-4} … $v_{n+i-(n-1)}$, $u_{n+i-(n-1)}$.

Hence the claim.

There are $\binom{n}{2}$ pair of vertices in $V(CL_{n.})$ such that the detour distance between them is $2n$-1.

Therefore $\omega(G) = \sum_{\{u,v\} \subset V(G)} l(u,v) = \binom{n}{2}(2n-1) = 4n^3 - 4n^2 + n$.

IV. Conclusion

Computation of detour index is challenging and *NP*-Complete problem. There are many research papers on the name of Wiener index has appeared in the literature but very limited number of papers on the name of detour index are available. This is due to the complexity of finding detour index. We have different technique available to compute Wiener index whereas no particular technique or method is available for Detour index. In this paper we represent an exact expression of detour index of circular ladder CL_n, n odd. Computation of circular ladder n even case is under investigation.

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