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ON DIAMETER OF $TUC_4C_8(S)[P,Q]$ LATTICE TITLE

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ABSTRACT. In this paper we consider a TUC4C8(S)[p,q] nanotube lattice where $q = kp$ and we compute its diameter.

Keywords: *TUC4C8 (S)[p,q] Nanotube lattice, Diameter of graph, Dual graph*

INTRODUCTION

Let G be a molecular graph with $V(G)$ and $E(G)$ being the set of atoms/vertices and bonds/edges, respectively. The distance between vertices u and v of G is denoted by $d(u,v)$ and it is defined as the number of edges in a path with minimal length connecting the vertices u and v.

A topological index is a numerical quantity derived in an unambiguous manner from the structural graph of a molecule and it is a graph invariant.

The Wiener index of a graph represents the sum of all distances in the graph. Another index, the Padmakar-Ivan (PI) index, is defined as $PI(G) = \Sigma[n_{eu}(e|G) + n_{ev}(e|G)]$, where $(n_{eu}, e|G)$ is the number of edges of *G* lying closer to *u* than to *v*, and $(n_{ev}, e|G)$ is the number of edges of *G* lying closer to *v* than to *u* and summation goes over all edges of *G*. Also, the Szeged index of a graph G is defined as $Sz(G) = \sum_{e\in E(\Gamma)} n_1(e \mid G) \cdot n_2(e \mid G)$, where $n_i(e \mid G)$ is the number of elements in

$$N(e \mid G) = \{x \in V(G) \mid d(u,x) < d(v,x)\} \text{ and } e = \{u,v\} \in E(G).$$

For $G = TUC_4C_8(S)[p,q]$ nanotubes (Figure1) the Wiener W, Padmakar-Ivan PI and Szeged Sz indices are topological indices that have been computed in refs. [1-5].

One important application for graphs is to model computer networks or parallel processor connections. There are many properties of such networks that can be obtained by studying the characteristics of the graph models. For example, how do we send a message from one computer to another by using the least amount of intermediate nodes? This question is answered

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by finding a shortest path in the graph. We may also wish to know what is the largest number of communication links required for any two nodes to talk with each other; this is equivalent to find the diameter of the graph.

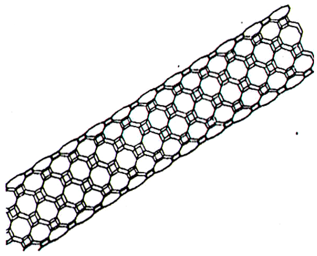

Figure 1: $G = TUC_4C_8(S)[p,q]$ Nanotube

Let $G = TUC_4C_8(S)[p,q]$ lattice (Figure 2) be a trivalent decoration made by alternating squares C_4 and octagons C_8. In [4] the diameter of a zig-zag polyhex lattice have been computed; in this paper the formula for the diameter of a $G = TUC_4C_8(S)[p,q]$ lattice will be derived.

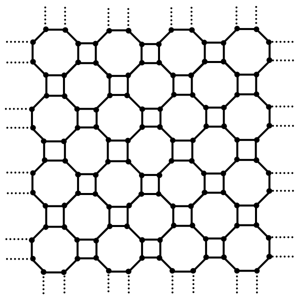

Figure 2: TUC_4C_8 lattice

RESULTS AND DISCUSSION

In this section we compute the diameter of the graph $G = TUC_4C_8(S)[p,q]$ where $q = kp$ and k, p are positive integers.

Definition 1. In $G = TUC_4C_8(S)[p,q]$ with $p = q$ any vertices of degree 2 and all vertices of degree 3 which are adjacent to a vertex of degree 2 is called boundary vertices (see Figure 3); a vertex which is not a boundary vertex is called an interior vertex. The set of all boundary vertices of G are denoted by $B(G)$.

Lemma 1. Let $d = d(G)$ be the diameter of G. Then for any $v-w$ path of length d, we have $\{v,w\} \in B(G)$.

The Proof is given by Lemma 2 [4].

Lemma 2. Suppose B_ℓ and B_β are the sets of left side and right side boundary vertices of G, respectively. If we sort the vertices of these sets from up to down such that $B_\ell = \{u_1, u_2, \ldots, u_n\}$ and $B_\beta = \{v_1, v_2, \ldots, v_n\}$, then $d(u_1, v_n) = d(G)$.

Proof. We consider the inner dual of $G = TUC_4C_8(S)[p,q]$, (Figure 3)

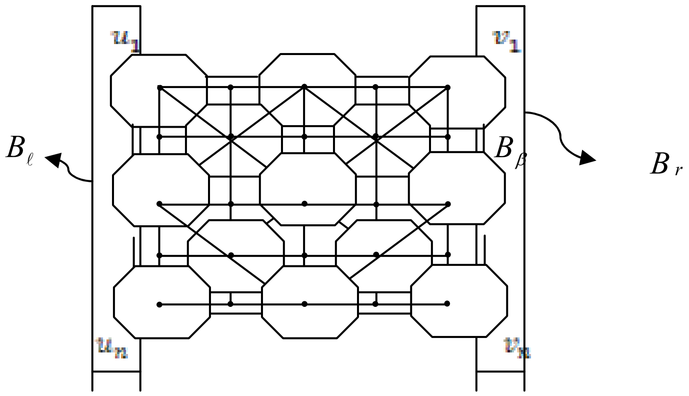

Figure 3: TUC_4C_8(S) lattice and its dual graph

Since

$$d(u_i, v_n) \leq d(u_1, v_n), \quad i = 1, 2, \ldots, n$$

and

$$d(u_n, v_i) \leq d(u_n, v_1), \quad i = 1, 2, \ldots, n$$

Then by symmetry of G we conclude that $d(G) = d(u_1, v_n) = d(u_n, v_1)$.

Theorem 1. Let $G = TUC_4C_8(S)[p,q]$, where $q = p$ and p, q are positive integers. Then we have $d(G) = 5p - 1$.

Proof. The proof is by induction on p. In case $p = 1$, G is an octagon with diameter 4 and the theorem is obviously true. Suppose that the theorem is true for the case $p = q = n - 1$ and consider a TUC_4C_8(S) [p,q] lattice of size $n \times n$. By Lemma 2, we have $d(G) = d(u_1, v_n)$. If we delete the last two rows and columns it is easy to see that $d(u_1, v_n) = d(u_1, v_{n-1}) + d(v_{n-1}, v_n)$. Hence,

$$d(G) = [5(n-1) - 2] + 6 = 5p - 1.$$

Theorem 2. Let, $G = TUC_4C_8(S)[p,q]$, where $q = kp$ and p, q are positive integers. Then we have $d(G) = (4k+1)p - 1$.

Proof. We prove the theorem by induction with respect to k. As *we* have seen for Theorem 1, the assertion is true for $k = 1$. Let $k > 1$ and suppose that the theorem is true for $q = kp$. Now consider a $G = TUC_4C_8(S)[p,q]$, lattice with $q = (k+1)p$. We may assume that the lattice contains $k + 1$ blocks

$B_1, B_2, \dots, B_{k+1}$ of $G = TUC_4C_8(S)[p,q]$ lattice each of size $(p\times p)$. Obviously it is enough to find the length of shortest path from vertex u_{11} to vertex $v_{(k+1)(p+1)}$.

By symmetry of $G = TUC_4C_8(S)[p,q]$ lattice, we conclude that $d(G) = d(u_{11}, v_{kp}) + d(v_{kp}, v_{(k+1)(p+1)}) = d(u_{11}, v_{kp}) + 4k + 2$.
Hence $d(G) = (4k+1)p - 1$.

EXAMPLES

In this section, we give some examples in the following tables. The diameter calculations were done by the TOPO-CLUJ software package [6]. In Table 1 we consider some special cases where $k = 1$, while in Table 2, we consider cases for $k > 1$.

Table 1. Some cases of $d(G)$ with $k = 1$.

p	$d(G)$	$5p - 1$
2	9	$5(2) - 1 = 9$
3	14	$5(3) - 1 = 14$
4	19	$5(4) - 1 = 19$

Table 2. Some cases of $d(G)$ with $k > 1$.

k	p	q	$d(G)$ (distance matrix)	$p(4k+1)-1$ (Theorem 2)
2	3	6	26	3(8+1)-1=26
3	3	9	38	3(12+1)-1=38
3	4	12	51	4(12+1)-1=51
4	3	12	50	3(16+1)-1=50
4	4	16	67	4(16+1)-1=67

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