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Augmented eccentric connectivity index of single-defect nanocones

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ABSTRACT. We present explicit formulas for the values of augmented eccentric connectivity indices of single-defect nanocones. Our main result is that the augmented eccentricity index of an n-layer nanocone with a single *k*-gonal defect at its apex behaves asymptotically $27k(1-\ln 2)n$ for $k \geq 5$.

Keywords: eccentricity, nanocone, augmented eccentric connectivity index.

1. INTRODUCTION

Single-defect nanocones are hypothetical nanostructures that arise by accretion of several layers of hexagons around a single non-hexagonal polygon. They can be obtained from the graphene lattice by introducing a non-hexagonal defect and inserting or removing the corresponding number of 60^0 sectors of hexagons. Defects with less than six sides introduce positive curvature; those with more than six sides result in a negative-curvature cone. The pentagonal nanocones have been actually

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generated and observed by Ge and Sattler in 1994 [6]. It has been long conjectured that they play an important role in the process of fullerene synthesis.

Single-defect nanocones posses a high degree of symmetry andregularity. That property facilitated explicit computation of several topological invariants, in particular those based on topological distances. Most of the results of such type were obtained by using the method of cuts; we refer the reader to a very informative survey [7] and references therein for more details. Another approach made use of the fact that certain distance-based invariants behave polynomialy in the number of vertices (or layers of hexagons) and allowed for explicit computation of such invariants by fitting. As an example, we mention recent papers on the eccentric connectivity index of single-defect nanocones [1, 8] and papers dealing with some distance-based invariants of several types of lattices [2, 3].

The main goal of this paper is to compute the augmented eccentric connectivity index of general single-defect nanocones. For that invariant neither of the mentioned approaches can be exploited, since the distances involved appear in denominators, resulting in a nonpolynomial behavior. Our results are closed formulas in terms of digamma function of a linear combination of two defining parameters, the size k of the non-hexagonal defect at the apex and the number n of layers of hexagons around it. It turns out that for large nanocones the augmented eccentric connectivity index behaves asymptotically as a linear function of n.

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2. DEFINITIONS AND PRELIMINARIES

Let *G* be a graph on p vertices. We denote the vertex and the edge set of *G* by V(*G*) and E(*G*), respectively. For two vertices *u* and *v* of V(*G*) we define their distance *d*(*u*, *v*) as the length of any shortest path connecting *u* and *v* in *G*. For a given vertex *u* of V(*G*) its eccentricity $\varepsilon(u)$ is the largest distance between *u* and any other vertex *v* of *G*. Hence, $\varepsilon(u) = \max_{v \in V(G)} d(u,v)$. The maximum eccentricity over all vertices of G is called the diameter of *G* and denoted by *D*(*G*); the minimum eccentricity among the vertices of *G* is called the radius of *G* and denoted by R(*G*). The set of all vertices of minimum eccentricity is called the center of *G*.

The augmented eccentric connectivity index ${}^{A}\xi(G)$ of a graph G is defined as

$$ {}^{A}\xi(G) = \sum_{u \in V(G)} \frac{M(u)}{\varepsilon(u)}, $$

where $M(u)$ denotes the product of degrees of all neighbors of vertex u. It was introduced in a paper [5] concerned with various modi ications of the eccentric connectivity index. We can see that the vertex contributions are both nonlocal (the degrees are taken over the neighborhoods and then multiplied) and non-linear in $\varepsilon(u)$. The combination of those two properties makes the augmented eccentric connectivity index rather unyielding to the standard approach to distance-based invariants, resulting in a number of difficulties arising when one tries to obtain explicit formulas or find the extremal graphs and values.

A single-defect k-gonal nanocone is obtained by taking a cycle on k vertices C_k and

surrounding it by certain number of concentric layers of hexagons so that all internal vertices are of degree 3. If there are n layers of hexagons, we denote such graph by $CNC_k[n]$.

For n = 0 we obtain just the k-gon C_k. An example is shown in Fig. 1. Obviously, for all $k \geq 3$, $CNC_k[n]$ is a planar graph with one k-gonal and $k\binom{n+1}{2}$ hexagonal faces.

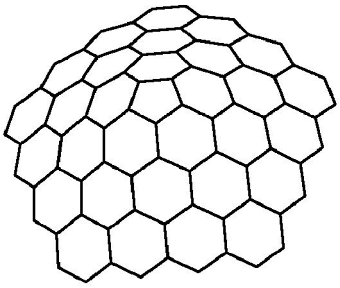

Fig. 1: A single-defect nanocone with pentagonal apex.

We consider in this paper only the case $k \geq 5$. The reason is that the eccentricities of vertices in such nanocones behave in a very regular way. The remaining two cases, $k = 3$ and $k = 4$, are also less interesting from the chemical point of view, since carbon atoms do not readily form short cycles.

It is easy to show by induction on n that there are exactly $(2n+1)k$ external vertices

in $CNC_k[n]$. (A vertex is external if it lies on the boundary of the unbounded face of $CNC_k[n]$; otherwise, the vertex is called internal.) An immediate consequence is the formula for the number of vertices in $CNC_k[n]$.

Proposition 1.

$$|V(CNC_k[n])| = k(n+1)^2 .$$

Further, we observe that there are four types of vertex neighborhoods in CNCk[n]. For all internal vertices, the product of their neighbors' degrees is equal to 27. Then, there are nk external vertices of degree 3; for all of them, $M(u)=12$. There are exactly $2k$ external vertices of degree 2 whose neighbors are of degree 2 and 3, and finally, there are $(n-1)k$ vertices of degree 2 whose both neighbors are of degree 3.

3. MAIN RESULTS

Throughout this section we assume $k \geq 5$. It is obvious from the symmetry argument that the center of CNCk[n] is made of the vertices of the central k-gon. Their eccentricities (and hence the radius of CNCk[n]) are equal to $\left\lfloor \frac{k}{2} \right\rfloor + 2n$. The claim follows directly by induction on n. By the same inductive argument it follows that the eccentricities of vertices increase by 2, 3, or 4 with each new layer of hexagons. This results in the following bounds on the eccentricity $\varepsilon(u)$ of a vertex u of CNCk[*n*].

Proposition 2.

Let u be a vertex of CNCk[*n*] for some $k \geq 5$. Then

$$\left\lfloor \frac{k}{2} \right\rfloor + 2n \leq \varepsilon(u) \leq \left\lfloor \frac{k}{2} \right\rfloor + 4n.$$

Hence, the eccentricities of vertices start at $\left\lfloor \frac{k}{2} \right\rfloor + 2n$ and increase by one till they reach $\left\lfloor \frac{k}{2} \right\rfloor + 4n$. The next task is to find the number of vertices of a given eccentricity. Again, by simple symmetry and counting arguments, we obtain the following result.

Proposition 3.

The number of vertices of CNCk[*n*] with the eccentricity equal to $\left\lfloor \frac{k}{2} \right\rfloor + 2n + j$ is equal to $k\left\lfloor \frac{j}{2} \right\rfloor + 2n$.

Now we have all the elements necessary for computing ${}^{A}\xi(CNC_k[n])$. It is clear that the contribution of external vertices will be marginal in comparison with the contribution of internal vertices. Indeed, the total contribution of external vertices is given by

$$E(n,k) = \frac{12kn}{\left\lfloor \frac{k}{2} \right\rfloor + 4n - 1} + \frac{3k(3n+1)}{\left\lfloor \frac{k}{2} \right\rfloor + 4n}.$$

The first term on the right-hand side comes from the vertices of degree 3, and the second term from the two types of vertices of degree 2.

The total contribution of internal vertices is obtained by summing over $j \in [0, 2n-2]$ of terms of the form $\frac{k(\left\lfloor \frac{j}{2} \right\rfloor + 1)}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + j}$ multiplied by $M(u) = 27$. The sum in the resulting expression

$$27k \sum_{j=0}^{2n-2} \frac{\left\lfloor \frac{j}{2} \right\rfloor + 1}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + j}.$$

can be expressed as

$$\sum_{j=0}^{2n-2} \frac{\left\lfloor \frac{j}{2} \right\rfloor + 1}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + j} = \sum_{j=1}^{n} \frac{j}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + 2j - 2} + \sum_{j=1}^{n-1} \frac{j}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + 2j - 1}.$$

The sums in the right-hand side can be expressed in terms of digamma function,

$$\sum_{j=1}^{n} \frac{j}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + 2j - 2} = \frac{n}{2} + \frac{2n + \left\lfloor \frac{k}{2} \right\rfloor - 2}{4} \left(\psi(n + \frac{\left\lfloor \frac{k}{2} \right\rfloor}{2}) - \psi(2n + \frac{\left\lfloor \frac{k}{2} \right\rfloor}{2}) \right);$$

$$\sum_{j=1}^{n-1} \frac{j}{\left\lfloor \frac{k}{2} \right\rfloor + 2n + 2j - 1} = \frac{n-1}{2} + \frac{2n + \left\lfloor \frac{k}{2} \right\rfloor - 1}{4} \left(\psi(\frac{2n + \left\lfloor \frac{k}{2} \right\rfloor + 1}{2}) - \psi(\frac{4n + \left\lfloor \frac{k}{2} \right\rfloor - 1}{2}) \right).$$

Here $\psi(x)$ denotes the digamma function, defined as the logarithmic derivative of the gamma function, $\psi(x)=\dfrac{\Gamma'(x)}{\Gamma(x)}$.

Now we could write down the formula for the augmented eccentric connectivity index of a general nanocone with single k-gonal defect at its apex. However, the resulting expression would be quite unwieldy; we leave the task to the interested reader. Instead, we will try to extract the information relevant for the asymptotic behavior. Crucial is the observation that the differences of digamma functions on the right-hand side of the obtained formulas tend to $-\ln 2$ for large values of n. By expanding the above expressions into a power series around ∞ we obtain

$$27k\sum_{j=0}^{2n-2}\frac{\left\lfloor \frac{j}{2}\right\rfloor+1}{\left\lfloor \frac{k}{2}\right\rfloor+2n+j}=27k\left[(1-\ln 2)n+\frac{1}{8}-\frac{1}{4}\ln 2\right]+O(\frac{1}{n}).$$

Now, by taking into account that $E(n,k)\approx\frac{21}{4}k$, we obtain the asymptotic behavior of ${}^{A}\xi(CNC_k[n])$.

Proposition 4.

$${}^{A}\xi(CNC_k[n])=27k\left[(1-\ln 2)n-\frac{1}{4}\ln 2\right]+\frac{69}{8}k+O(\frac{1}{n}).$$

Hence, the augmented eccentric connectivity index of a single-defect nanocone increases linearly with the number of hexagon layers. It means that it behaves proportionally to the square root of the number of vertices. For the two most interesting cases, the pentagonal nanocone $CNC_5[n]$ and the "flat" nanocone $CNC_6[n]$ we obtain the asymptotic behavior of the form ${}^{A}\xi(CNC_5[n])\approx 41.4251n+19.7313$ and ${}^{A}\xi(CNC_6[n])\approx 49.7102n+23.6775$, respectively. The quality of approximation is illustrated by the fact that the approximate value of 433.983 is quite close to the exact value of ${}^{A}\xi(CNC_5[10])=433.238$.

4. CONCLUDING REMARKS

In this paper we have determined the behavior of the augmented eccentric connectivity index of general single-defect nanocones. It was found that it behaves linearly in the number of hexagon layers for large values of n. It would be interesting to extend the present results to the case of cones with multiple defects and to the cones resulting from introducing defects into other regular tilings of the plane. The approach used here could be also suitable for computing augmented eccentric connectivity indices of narrow hexagonal nanotubes, of tubular fullerenes and of reticular benzenoid graphs such as those considered in [4].

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