Research Article

Süleyman Ediz* and İdris Çiftçi#

On *k*-regular edge connectivity of chemical graphs

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Abstract: Quantitative structure property research works, which are the essential part in chemical information and modelling, give basic underlying topological properties for chemical substances. This information enables conducting more feasible studies between theory and practice. Connectivity concept in chemical graph theory gives information about underlying topology of chemical structures, fault tolerance of molecules, and vulnerability of chemical networks. In this study we first defined two novel types of conditional connectivity measures based on regularity notion: k-regular edge connectivity and almost k-regular edge connectivity in chemical graph theory literature. We computed these new graph invariants for cycles, complete graphs, and Cartesian product of cycles. Our results will be applied to calculate k-regular edge connectivity of some nanotubes which are stated as Cartesian product of cycles. These calculations give information about fault tolerance capacity and vulnerability of these chemical structures.

Keywords: chemical graph theory, connectivity, conditional connectivity, k-regular edge connectivity, almost k-regular connectivity

1 Introduction

Quantitative structure property relationship/quantitative structure activity relationship research works involve graph theoretical analysis of chemical substances. These investigations enable to predict physical and chemical properties of chemical substances without conducting very expensive experimental studies. These studies also give the knowledge of the underlying topology of the molecules.

The fault tolerance of a chemical network is an important measure to conduct reliable studies in view of chemical information and modelling. Connectivity notion in graph theory is one of the leading means determining fault tolerance of chemical networks. But classical connectivity is not enough to determine fault tolerance and vulnerability of chemical networks since it assumes every atom has equivalent role in chemical point of view. To handle this problem, Harary posed conditional connectivity notion in graph theory (Harary, 1983). There are special desired properties held in all remaining components for conditional connectivity measurement. After that, many conditional connectivity measures were defined in the literature such as cycle-edge connectivity, restricted connectivity, extra connectivity, structure connectivity etc. Restricted connectivity was defined by Esfahanian and Hakimi (1988). Extra connectivity was initiated by Fabrega and Fiol (1996). Super-connectivity and super-edge-connectivity for some interconnection networks were investigated by Chen et al. (2003). Restricted h-connectivity measures for large multiprocessor systems were studied by Latifi et al. (1994). Structure connectivity and substructure connectivity of hypercubes were defined by Lin et al. (2016). The following references are the latest studies of these different conditional connectivity measurements: Cheng (2022), Gao et al. (2022), Guo et al. (2022), and Soliemany et al. (2022).

Regularity, which is a desired notion in chemical graph theory, is an important parameter in view of chemical network science especially in nanotubes. We decided to define novel conditional connectivity measurements because of lack of regularity-based conditional connectivity in graph theory literature. We first introduced two novel connectivity measurement notions in (chemical) graph theory literature: k-regular edge connectivity and almost k-regular edge connectivity. We computed both these novel conditional connectivity notions for cycles, complete

This study is based on the second author's PhD thesis.

* **Corresponding author: Süleyman Ediz,** Department of Mathematics, Faculty of Education, Van Yüzüncü Yıl University, Van, Turkey, e-mail: suleymanediz@yyu.edu.tr
İdris Çiftçi: Department of Mathematics, Faculty of Education, Van Yüzüncü Yıl University, Van, Turkey, e-mail: idrisciftci@yyu.edu.tr

graphs, and Cartesian product of cycles. Our results will be applied to calculate k-regular edge connectivity of some chemical nanotubes which are stated as Cartesian product of cycles. These calculations give information about fault tolerance capacity of these chemical structures.

2 Materials and method

Necessary definitions are given in order to prepare the reader for calculations of the k-regular edge connectivity and almost k-regular connectivity.

Let $G = (V, E)$ be a connected graph where V is the vertex set and E is the edge set. The degree of any vertex (atom and node) of G is the number of edges (bond and link) incident to this vertex and denoted as deg v for the vertex v of V. If a graph has maximum degree of at most four, then it is called chemical graph. If all the degrees of the vertices of G equal r, then G is called r-regular graph. A 3-regular graph is named as cubic graph. 2-regular connected graphs with n-edge and n-vertex are called cycles and denoted as C_n. If an edge is deleted from the cycle C_n, then the path graph P_n is acquired. In an n-vertex graph, if every vertex is adjacent to all the other vertices, then this graph is called complete graph and denoted as K_n. Let G and H be two simple connected graphs, then Cartesian product of these graphs, denoted as $G \times H$, is characterised by its vertex set $V(G \times H) = V(G) \times V(H)$ and the edge set $E(G \times H) = \{(g_1, h_1)\ (g_2, h_2) | \text{either } g_1 = g_2,\ h_1h_2 \in E(H) \text{ or } h_1 = h_2,\ g_1g_2 \in E(G)\}$.

In edge connectivity of a connected graph G, $\lambda(G)$ is the minimum number of edges whose deletion makes the graph G disconnected.

And now we first give the definitions of two novel conditional connectivity measures in (chemical) graph theory: k-regular edge connectivity and almost k-regular edge connectivity. Let G be a graph and S be a set of edges. If G-S is disconnected and each component is a k-regular graph, then S is called a k-regular edge cut of G. The minimum cardinality of a k-regular edge cut of G is called k-regular edge connectivity of G and denoted as $\lambda^{kr}(G)$.

Similar definition can be given for almost k-regular connectivity of G. Let G be a graph and S be a set of edges. If G-S is disconnected and $|\deg u - \deg v| \leq k$ for any two vertices belong to any disconnected component, then S is called an almost k-regular edge cut of G. The minimum cardinality of an almost k-regular edge cut of G is called almost k-regular edge connectivity of G and denoted as $\lambda^{akr}(G)$. We use the symbol □ to indicate that the proof is completed.

And now we begin to compute the k-regular edge connectivity and almost k-regular edge connectivity for cycles, and complete graphs as well as Cartesian product of cycles.

We use combinatorial computing techniques and methods in our computations.

3 Results

In this section, we first compute k-regular edge connectivity and almost k-regular edge connectivity for cycles, complete graphs, and Cartesian product of paths and cycles. The following observations are direct consequences of definition of k-regular edge connectivity notion.

Observation 1
$\lambda^{1r}(C_n) = \frac{n}{2}$ for any even number for $n \geq 4$.

Proof. Every disconnected component must be isomorphic to K_2 after the application of the definition for 1-regular edge connectivity. Thus, suitable but not neighbouring edges deletion gives the result directly. □

Observation 2
$\lambda^{1r}(K_n) = \frac{n(n-2)}{2}$ for any even number for $n \geq 4$.

Proof. As in the proof of Observation 1, we want to get $\frac{n}{2}$ number of disconnected K_2 after the application of 1-regular edge connectivity definition. We know that K_n has $\frac{n(n-1)}{2}$ edges. Therefore, it must be necessary to delete $\frac{n(n-2)}{2}$ suitable edges. □

Observation 3
$\lambda^{2r}(K_n) = \frac{n(n-3)}{2}$ for any integer for $n \geq 4$.

Proof. We must disconnect K_n into at least two cycle components. Let these disconnected components be C_3 and C_{n-3}. The number of all edges are $2n$ in C_3 and C_{n-3}. Therefore, deletion of $\frac{n(n-3)}{2}$ suitable edges gives the result. □

Observation 4
$\lambda^{3r}(K_n) = \frac{n(n-4)}{2}$ for any even number for $n \geq 8$.

Proof. We must disconnect K_n into at least two components such that both of them are 3-regular graphs. Without loss of generality we assume that one of the disconnected component graphs is K_4 and the other disconnected graph is 3-regular graph with $n-4$ vertices. The number of all edges are $\frac{3n}{2}$ in both the disconnected components. Therefore, the deletion of $\frac{n(n-4)}{2}$ suitable edges gives the result. □

Observation 5
$\lambda^{4r}(K_n) = \frac{n(n-5)}{2}$ for any integer for $n \geq 10$.

Proof. We must disconnect K_n into at least two components such that both of them are 4-regular graphs. Without loss of generality, we assume that one of the disconnected component graphs is K_5 and the other disconnected graph is the 4-regular graph with $n-5$ vertices. The number of all edges are $2n$ in both the disconnected components. Therefore, the deletion of $\frac{n(n-5)}{2}$ suitable edges gives the result. □

And now we can give the generalisation formula for computing k-regular edge connectivity of complete graphs with suitable n and k.

Theorem 1. $\lambda^{kr}(K_n) = \frac{n(n-k-1)}{2}$ *for suitable integers n and k.*

Proof. We must disconnect K_n into at least two components such that both of them are k-regular graphs. Without loss of generality, we assume that one of the disconnected component graphs is K_{k+1} and the other disconnected graph is k-regular graph with $n-k-1$ vertices. The number of all edges are $\frac{kn}{2}$ in both the disconnected components. Therefore, deletion of $\frac{n(n-k-1)}{2}$ suitable edges gives the result. □

Observation 6

$$\lambda^{a1r}(C_n) = 2$$

Proof. We get disconnected two paths after the deletion of two non-neighbour edges from C_n. Notice that the difference in degrees for any two vertices in every two different components is equal to one or smaller than one. That is, the difference inequality condition holds which is stated in the definition of almost 1-regular edge connectivity notions. □

Proposition 1.

$$\lambda^{a1r}(K_n) = 2n - 4$$

Proof. We know from the definition of almost 1-regular edge connectivity that we want to disconnect K_n into at least two disconnected graphs such that the difference in degrees for any two vertices in every two different components are equal to one or smaller than one. Without loss of generality, these two disconnected components must be K_2 and K_{n-2} in order to delete minimum number of suitable edges. Thus, it is necessary to delete at least $2(n-2)$ edges. And this gives the result. □

Corollary 1. $\lambda^{akr}(K_n) = 2n - 4$ *for* $n \geq 7$ *and* $1 \leq k \leq n-1$.

Proof. The proof is the same as that of Proposition 1. □

And now we begin to investigate k-regular edge connectivity for Cartesian products of paths and cycles. We know from the definition of 1-regular edge connectivity that if a connected simple graph has odd number of vertices, then it is not possible to disconnect this graph into disconnected K_2 components. Therefore, we assume that the following graphs, which are the Cartesian products of paths and cycles, always must have even number of vertices. The Cartesian product of paths are called as complete grid graphs. The Cartesian product of $P_5 \times P_6$ is depicted in Figure 1.

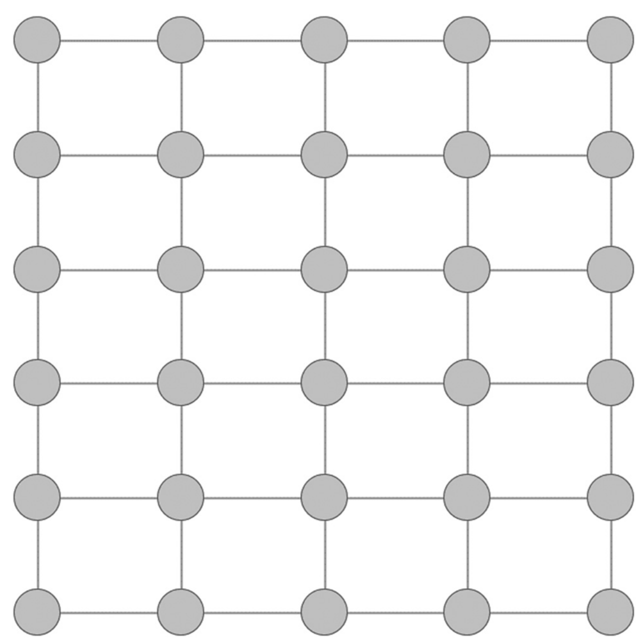

Figure 1: The Cartesian product graph of $P_5 \times P_6$.

Proposition 2. *Let P_m and P_n be two paths with m being odd and n being even. Then, 1-regular edge connectivity of the Cartesian product of these paths is $\lambda^{1r}(P_m \times P_n) = \frac{3mn}{2} - m - n$.*

Proof. Without loss of generality, if we assume that n is odd and m is even, then we acquired the same graph since we know that $P_m \times P_n$ is isomorphic to $P_n \times P_m$ from the definition of the Cartesian product of graphs. It is seen that $P_m \times P_n$ has $(m-1)n$ edges horizontally and $m(n-1)$ edges vertically from Figure 1. Our aim is to delete enough number of edges vertically and horizontally from $P_m \times P_n$ such that every disconnected component is isomorphic to K_2. Therefore, we must delete all $(m-1)n$ horizontal edges and $\frac{n-2}{2}m$ vertical suitable edges. Thus, total value of the deleted edges equals $\frac{3mn}{2} - m - n$. □

Proposition 3. *Let P_m and P_n be two paths with m and n being even. Then, 1-regular edge connectivity of the Cartesian product of these paths is $\lambda^{1r}(P_m \times P_n) = \frac{3mn}{2} - m - n$.*

Proof. Deletion of non-neighbouring suitable $\frac{m-2}{2}n$ number of horizontal edges and $\frac{n-2}{2}m$ number of vertical edges gives disconnected $\frac{mn}{4}$ number components which are isomorphic to C_4 in $P_m \times P_n$. We know that deletion of two non-neighbour edges in C_4 gives two disconnected components which are isomorphic to K_2. Therefore, deletion of $2\frac{mn}{4} = \frac{mn}{2}$ edges in all C_4 gives two disconnected components which are isomorphic to K_2. Thus, total value of deleted edges equals $\frac{m-2}{2}n + \frac{n-2}{2}m + \frac{mn}{2} = \frac{3mn}{2} - m - n$. □

Proposition 4. *Let C_m and C_n be two cycles where at least one of m or n is even. Then, 1-regular edge connectivity of the Cartesian product of these paths is $\lambda^{1r}(C_m \times C_n) = \frac{3mn}{2}$.*

Proof. The Cartesian product graph $C_m \times C_n$ has $m + n$ extra edges than the Cartesian product graph $P_m \times P_n$. We know that $\lambda^{1r}(P_m \times P_n) = \frac{3mn}{2} - m - n$ from Propositions 2 and 3. We proceed in the same way as in the proofs of Propositions 2 and 3. Therefore, it is enough to delete this $m + n$ extra edges from the Cartesian product graph $C_m \times C_n$, to get 1-regular edge connectivity of $C_m \times C_n$. Thus, $\lambda^{1r}(C_m \times C_n) = \frac{3mn}{2}$. □

Proposition 5. *Let C_m and C_n be two cycles. Then, 2-regular edge connectivity of the Cartesian product of these cycles is $\lambda^{2r}(C_m \times C_n) = mn$.*

Proof. We want to get disconnected components all of which are isomorphic to either C_m or C_n. From the help of the Cartesian product of $P_m \times P_n$, we know that the Cartesian product graph $C_m \times C_n$ has $m + n$ extra edges than the Cartesian product graph $P_m \times P_n$. We consider two cases separately.

Case 1

We want to get disconnected components all of which are isomorphic to C_m. We must delete n vertical edges of every row. The number of rows in $C_m \times C_n$ is m. Therefore, we need to delete mn edges in total.

Case 2

We want to get disconnected components all of which are isomorphic to C_n. We must delete m horizontal edges of every column. The number of columns in $C_m \times C_n$ is n. Therefore, we need to delete mn number of edges in total.

There are many nano-molecules which they are stated as Cartesian product of chemical graphs. Therefore, our results have been used to compute fault tolerance and vulnerability parameters for chemical graphs in view of k-regular edge connectivity. □

4 Conclusion

Conditional connectivity measures give information about fault tolerance and vulnerability of chemical molecules. This information enables to conduct more feasible studies in view of chemical information and modelling. The main focus of this study is to define two novel conditional connectivity invariants based on regularity notion in chemical graph theory: k-regular edge connectivity and almost k-regular connectivity, and to compute these novel chemical graph invariants' cycles, complete graphs, and Cartesian products of cycles. These calculations for Cartesian product of chemical graphs are essential for understanding fault tolerance and vulnerability parameters in these chemical networks. There are many novel research alternatives related about this study for example:

- Investigating k-regular edge connectivity of metal molecular structures,
- Computing k-regular edge connectivity of interconnection networks,
- Studying relationship between k-regular edge connectivity and the other conditional connectivity instruments,

- Calculating k-regular edge connectivity in graph operations,
- Reckoning k-regular edge connectivity for nanotubes which are stated via graph product.
- Defining k-regular vertex connectivity and computing molecular graphs.

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