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Graph Theory: Applications to Chemical Engineering and Chemistry

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ABSTRACT

Chemical and biochemical reaction engineering contains many complicated mechanisms. Many investigators have studied kinetic aspects of reactions. Also biochemical reactions are becoming important due to their advantages such as low activation energy and specificity. Many investigators have studied equivalence between chemical structures and graphical structures. The chemical formulae in chemistry resemble the graphical structures. Various papers based on graph theory related to scheduling concepts, computer science applications are also studied by investigators. The use graph theory in chemical engineering is very handy and effective tool. Current review summarizes research and studies on graph theory related to chemistry and chemical reaction engineering.

Key words: Covalent structure, chemical kinetics, equilibrium, mathematical chemistry.

INTRODUCTION

Chemical engineering is much diversified field. The essence of chemical engineering lies in physics, chemistry and mathematics. Chemical engineering subjects include chemical reactions, interaction between molecules, kinetic aspects and isotherms. Chemical and biochemical reaction engineering contains many complicated mechanisms. Many investigators have studied kinetic aspects of reactions. [1-4] Also biochemical reactions are becoming important due to their advantages such as low activation energy and specificity. [5-8] Many investigators have studied equivalence between chemical engineering and mathematics. The formulae writing in chemistry resembles the graphical structures. The use graph theory in chemical engineering is very handy and effective tool. Current review summarizes research and studies on graph theory.

GRAPH THEORY: APPLICATIONS TO CHEMICAL ENGINEERING AND CHEMISTRY

Prathik et.al. studied the applications of graph theory. [9] They found that graph theory has wide applications in biochemistry, chemistry, communication networks and coding theory, computer science (algorithms and computation) and operations research (scheduling). They studied various papers based on graph theory related to scheduling concepts, computer science applications. They discussed importance of graphs in chemistry. The covalent structures are constitutional graphs only. Other graph problems in graph theories, according to them, are defining and finding the constitutional isomers. They also observed that data mining also uses graph theory to a great extent. Other applications included finger print classification, Job scheduling etc. Balaban compared the graph theory with Sherlock Holmes Principle. [10] According to them, the method in which, we find all graphs fulfilling certain mathematical conditions and then eliminate chemically impossible solutions, resemble Sherlock Holmes Principle. He presented centered on chemical applications of graph theory including an overview of the interactions between chemistry and discrete mathematics. He prepared equivalence between chemical and mathematical terms. The constitutional formulae were explained in view of Sherlock Homes principle, "When you have eliminated the impossible, whatever remains, no matter how improbable, must contain the truth".

Balaban discussed applications of graph theory in chemistry. [11] He dealt with definition, enumeration, and systematic coding or nomenclature of constitutional or steric isomers. According to him, Pauli's principle, Polya's theorem and electro negativities can be combined to explore all possible monocyclic aromatic and hetero-aromatic compounds. Also he discussed applications of graph theory in chemical nomenclature (nodal nomenclature and related areas), coding and information processing/storage/retrieval. Estrada, in his chapter from the book discussed chemical graph theory (CGT). [12] A branch of mathematical chemistry which deals with the nontrivial applications of graph theory to solve molecular problems was defined as chemical graph theory. He noted that a chemical structure is graph with the atoms as the vertices of the graph and the molecular bonds as the edges. The CGT in mainly used to reduce the topological structure of a molecule to a single number. Bapodra discussed ordinary differential equations for a chemical reaction, using graph transformation techniques. [13] He also presented summary of relevant graph transformation theory used in the project. He experimented with many variations for suitable molecular representation necessary to specify molecules and their reactions. Heck discussed method for graphically modeling chemical kinetics. [14] According to him, use of system dynamics modeling software can help to develop students' knowledge about chemical kinetics and chemical equilibrium. According to him, It can also remediate alternative concept. For the modeling in chemical kinetics, he also discussed methodology, strengths, and weaknesses of the implementation of graphical system dynamics software. In cases of non-trivial reaction mechanisms, graph theory, according to him will represent thinking of a chemical engineer. Chemical reaction networks were analyzed by using graph theory by Othmer. [15] He determined the dynamical behavior of a chemically-reacting system. For this purpose, he used the stoichiometry of the reactions, the structure of the graph underlying the network, and the reaction phenomenology embodied in the rate laws. He proposed a new approach to the analysis of networks. His approach was aimed at avoiding the individual influences to the extent possible, and facilitates the analysis of their interaction. According to his studies, a network of positive deficiency is dynamically equivalent to one with zero deficiency. Shiu discussed the algebraic study of chemical reaction networks. [16] The networks were endowed with massaction kinetics. He also developed basic theory of toric dynamical systems. These are the reactions where the amount produced is equal to the amount consumed. He also discussed the concept of Siphons. These are subsets of the chemical species that have the potential of being absent in a steady state. Callaghan discussed graphical approach for kinetics and catalysis of the water-gas-shift reaction(WGS) along with a microkinetic approach. [17] In his investigation, he proposed a comprehensive predictive micro-kinetic model for the WGS reaction. According to him, to graphically depict and analyze reaction mechanisms, reaction route graph theory is handy tool. A series of routes by which the reactants may be converted to products can be represented by reaction route graph theory. He believed that route reaction graph theory is invaluable for unraveling the mechanism and kinetics of complex catalytic reactions. Studies were carried out by Bournez et.al. for automated generation of kinetic chemical mechanisms. [18] They used the rewrite system ELAN for the automated generation of the combustion reactions mechanisms. They advocated importance of rewriting and rule-based programming. According to Domijan, it is crucial to understand the underlying chemical reactions for understanding biological processes. [19] He pointed out that graph theory can be applied where models for which other techniques fail. He reviewed some of the most recent graph theory that

has been applied to studies of chemical reaction networks (CRNs). Kvasnicka discussed first-order chemical kinetics. [20] He investigated the first-order reactions kinetics. He has shown that an arbitrary closed kinetic system of first-order reactions asymptotically tends to an equilibrium state. In turn, in this equilibrium step, all time derivatives of concentrations go vanishing. According to the studies carried out by Malik and Imran, the first and second Zagreb indices can be incorporated for study of anti-inflammatory activities of certain chemical instances. [21] In their work they calculated the Zagreb indices and the multiplicative versions of the Zagreb indices of an infinite class of titania nanotubes TiO_2. E. Davis and J. Davis discussed fundamental principles in chemical reaction engineering. [22] It can be observed that in many computations and analysis graphical solution is an integral part of the chemical reaction engineering. Hu et. al. reviewed the matrix expression, topological index and atomic attribute of molecular topological structure. [23] They listed limitations of topological indices such as in explicit physical-chemical meaning of topological index and difficulty in expression of Quantitative structure-activity relationships (QSAR) and quantitative structure- activity relationships (QSPR).They emphasized the need for detailed studies on inter-correlation of topological index.

CONCLUSION

Many investigators have studied equivalence between chemical structures and graphs. The formulae writing in chemistry resembles the graphical structures. Various papers based on graph theory related to scheduling concepts, computer science applications are studied. by investigators. The use graph theory in chemical engineering is very handy and effective tool. Current review summarized research and studies on graph theory in chemistry and chemical reaction kinetics and engineering.

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