

A Review on Computer Application in Chemical Engineering: A Brief Insight

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ABSTRACT

Chemical engineering subjects like reaction engineering, transport phenomenon, mass transfer and optimization contain very rigorous numerical and analytical data and equations. Many times the calculation from the equations and actual practical results are verified for consistency. Solving these equations manually is time-consuming and impractical. Many software tools are available for solving these problems. Unisim, MATLAB, Simulink, HYSYS are few such tools. Simulation and optimization of the data can be carried out by using the mathematical concepts combined with these tools. The current review summarizes research and studies on the application of computer and software in chemical engineering practice and teaching.

Keywords: Simulation, Optimization, Process, Modeling, Numerical Analysis.

I. INTRODUCTION

Chemical engineering is very vast and diversified area. It deals with material science, fluid flow, process engineering mass transfer, heat transfer, optimization, operation research and so many interdisciplinary subjects like thermodynamics and environmental engineering. In most of the under graduate studies, the computer application is an important subject. The advanced mass transfer operations include reactive distillation, reactive adsorption, reactive chromatography etc. [1-5]. Other advances include membrane separations, new catalyst development, and modification of existing processes [6-11].

Advances in allied subjects like environmental engineering and energy system design include various new approaches for optimization and environmental friendliness [12-15]. Chemical engineering subjects like reaction engineering, transport phenomenon, mass transfer and optimization contain very rigorous numerical and analytical data and equations. Many times the calculation from the equations and actual practical results are verified for consistency. Solving these equations manually is time-consuming and impractical. Many software tools are available for solving these problems. Unisim, MATLAB, Simulink,

HYSYS are few such tools. Simulation and optimization of the data can be carried out by using the mathematical concepts combined with these tools. The current review summarizes research and studies on the application of computer and software in chemical engineering practice and teaching.

II. COMPUTER APPLICATION IN CHEMICAL ENGINEERING

According to Klatt and Marquardt, process systems engineering (PSE) is a very important area of investigation for many years [16]. Methodologies and tools to support process modeling, simulation and optimization (MSO) have been the great achievement of this field. It is necessary to reassess and reposition its future research agenda. They assessed the status and the future perspectives of PSE from an academic as well as from an industrial point of view. According to them, PSE follows the systems engineering paradigm and targets at the analysis and synthesis of (chemical) process systems. PSE is one of the very important methodologies for chemical engineering decisions. For PSE, to maintain identity and increase the popularity it is necessary to have long-term research on the core expertise with a focus on model-based systems engineering methods. Bernard et.al. studied recent

developments in process design [17]. They focused on establishing optimization-based approaches to support decision-making under uncertainty. In their work, they developed an optimal design framework, which allowed to decide how much it is worth to spend in research and experimentation for selectively reducing parameter uncertainties and guiding R and D activities. They developed and tested a stochastic optimization framework for achieving optimal process design. They carried out the trade-off between economic added value derived from parameter uncertainty reduction and information costs associated with experiments and R and D efforts. For the case under their consideration, they found that conduction of selective experiments is advisable.

Niklasson et.al. examined changes in mathematics education with integration into engineering subjects[18]. According to them, more effective methodology involves teaching in smaller groups, more varied assessment and greater integration of mathematics and chemistry. According to them, realistic chemical engineering examples can be used for better understanding of the mathematical concepts. Their work was focused on the understanding of basic concepts along with algorithms. Links between subjects, schools, and courses needed to be developed. In traditional mathematics problem formulation and solution in chemical engineering subjects have is limited to analytical solutions. According to them, with a constructive approach, based on numerical computation, it is possible to address equations in their general form.

Kantor and Edgar discussed computing skills in the chemical engineering curriculum[19]. According to them, chemical engineering has become strongly dependent on computing. It is necessary to utilize computer-based methods in order to enhance students' problem-solving skills. Nonavailability of computer-based textbook is a key limitation in use of computer-based methods for solution. It is necessary to carry out various projects aimed at making computer tools available. According to the author, subjects such as transport, thermodynamics and separations can be taught with more insight into solving the problems with computer programming.

Schofield explored the possibility of use of virtual reality simulator technology for a chemical engineering

education application [20]. According to their investigations, the technology used for film and computer game industries can allow educational developers to rapidly create realistic online virtual environments. According to them, there are a large number of problems which require innovative solutions. They emphasized the fact that there are a number of issues and concerns that arise through the use of online VR-based learning environments. They expressed the need for further investigation to safeguards and avoid any possible misuse of the technology. Wong and Barford carried out a project aimed at teaching of user-friendly Excel Visual Basic for Application (VBA) programming in chemical engineering [21]. They discussed the method to convert a chemical engineering problem into a working program. They emphasized the importance of Excel Visual Basic for Application (VBA) programming in chemical engineering. They compared the VBA with other software for problem solving. Kumar discussed the use of computer programming in balancing chemical reaction [22]. He carried out a survey of 13 methods used for problem solving. 6 were matrix methods, 2 were interactive programs. 1 was a standalone system and 1 was developed in the algorithm in Basic. One more was based on design engineering, while another one was written in HyperCard. 1 prepared for the World Wide Web. They estimated a number of independent chemical reactions, calculate yields, predict mass relationships, and balance. Assis and Lopes discussed free software available for chemical engineering education [23]. According to them; free software idea encourages the cooperative work. They discussed the implications of the free software ideas in chemical engineering educational and professional career.

Cutlip and Satan presented a workshop on recent advances in chemical engineering problem solving[24]. They provided a basic overview of current capabilities of several software packages. They focused on three soft wares namely POLYMATH, Excel, and MATLAB. According to them, main objectives of process computations are, deriving the mathematical model of the physical phenomena and critically analyzing the results. A numerical software package can handle technical details. Manafov described the software package for the solution of a wide range of tasks of the chemical and petrochemical industry[25]. He analyzed existing programs and specified their shortcomings and advantages. According to them, the

two methods namely golden section and Brentopt's method are advantageous as they are quite simple, do not require large computing resources, and do not require the derivative of the objective function. Piya asks method also has a simple convergence condition and can be applied to a broad class of functions.

Cutlip and Shacham provided a collection of representative problems with detailed solutions that can be used to introduce numerical problem solving[26]. They focused on chemical engineering courses. According to them, in chemical engineering, it is necessary to use the numerical analysis areas of linear equations, nonlinear equations, ordinary differential equations, partial differential equations, and regressions with statistics. They demonstrated the use of software packages like Microsoft Excel, MATLAB, and Polymath.

III. CONCLUSION

Many software tools are available for solving these problems. Unisim, MATLAB, SimuLINK, HYSYS are few such tools. Simulation and optimization of the data can be carried out by using the mathematical concepts combined with these tools. According to investigators, in chemical engineering it is necessary to use the numerical analysis areas of linear equations, nonlinear equations, ordinary differential equations, partial differential equations, and regressions with statistics. It was found that with a constructive approach, based on numerical computation, it is possible to address equations in their general form.

IV. REFERENCES

- [1]. Sunil Jayant Kulkarni, "Advancements, Research and Challenges in Reactive Adsorption: A Review", International Journal of Research (IJR), Vol.2, No.1, pp.310-313, 2015.
- [2]. Guangzhong Li, Yang Yu, Peng Bai, "Batch Extractive Distillation of Mixture Methanol-Acetonitrile Using Aniline as A Solvent", Polish Journal of Chemical Technology, Vol.14, No.3, pp.48-53, 2012.
- [3]. Sunil Jayant Kulkarni, "Solar Distillation: A Review", International Journal of Research (IJR), Vol.1, No.11, pp.1171-1176, 2014.
- [4]. Sunil Jayant Kulkarni, "A Review on Research and Advancements in Extractive Distillation", International Journal of Research (IJR), Vol.2, No.1, pp.306-309, 2015.
- [5]. Sunil J. Kulkarni, Ajay Giri K. Goswami, Nilesh L. Shinde, "A Review on Use of Chromatography for Analytical Applications", International Journal of Scientific Research in Science, Engineering, and Technology (ijsrset.com), Vol.1, No.4, pp.283-285, 2015.
- [6]. Sunil J. Kulkarni, Ajaygiri K. Goswami, "Applications And Advancements In Treatment Of Waste Water By Membrane Technology- A Review", International Journal Of Engineering Sciences and Research Technology, Vol.3, No.9, pp.446-449, 2014.
- [7]. Rashmi Vinod Dahake, A.K.Goswami, Dr. V. Kalyanraman, S.J.Kulkarni, "Performance Evaluation Of Hybrid Membrane Bioreactor For Low Strength Wastewater Treatment", International Journal Of Science, Engineering And Technology Research (IJSETR), Vol.2, No.12, pp. 2167-2169, 2013.
- [8]. A.S. Khojare, A.B. Kadu,P.G.Wasnik,M.R. Patil and Mrs. B.A.Khojare,"Adaptability of Membranes for Dairy Waste Management", Asian J. Exp. Sci.,Vol. 19, No. 2, pp.105-112, 2005.
- [9]. Sunil Jayant Kulkarni, "A Review on Petroleum Refining and Petrochemical Processes with Special Emphasis on Catalysts and Flue Gas Treatment Technology", International Journal of Petroleum and Petrochemical Engineering (IJPPE), Vol. 2, No. 1, pp.1-5, 2016.
- [10]. Sunil Jayant Kulkarni, "Research on Biocatalysts: A Review", International Journal of Research, Vol.2, No.4, pp.784-789, 2015.
- [11]. Sunil J. Kulkarni, "A Review on Studies and Research on Catalysts with Emphasis on Catalyst Deactivation", International Journal of Research and Review, Vol.2, No.10, pp.610-614, 2015.
- [12]. Sunil J. Kulkarni, Jayant P. Kaware, "Packed Bed Adsorption Column Modeling for Cadmium Removal", Int. J. of Thermal & Environmental Engineering, Vol.9, No. 2, pp.75-82, 2015.
- [13]. Kulkarni SJ, Kherde PM., "A Review on Advanced Membrane Separation Methods for Water Treatment, Int. J Res Rev., Vol.2, No.8, pp.513-517, 2015.
- [14]. Veena Ramachandran,Tanmay Uttam Gound, Sunil Kulkarni, "Biofiltration For Waste Gas Treatment- A Review", International Journal Of

- Ethics In Engineering & Management Education, Vol.1, No.4, pp.8-13, 2014.
- [15]. Sunil J. Kulkarni And Jayant P. Kaware, "Modeling For Packed Bed Phenol Removal By Low Cost Adsorbent Prepared From Rice Husk", *Sci. Revs. Chem. Commun.*, Vol.6, No.1, pp.1-11, 2016.
- [16]. Karsten-Ulrich Klatt, Wolfgang Marquardt, "Perspectives For Process Systems Engineering—Personal Views From Academia And Industry", *Computers And Chemical Engineering*, Vol. 33, pp.536-550, 2009.
- [17]. Fernando P. Bernardo A, Pedro Saraiva A, Efstratios N. Pistikopoulos, "Inclusion of Information Costs in Process Design Optimization Under Uncertainty", *Computers And Chemical Engineering*, Vol. 24, pp.1695-1701, 2000.
- [18]. Claes Niklasson, Michael Christie, Stig Larsson, Lars Ohrstrom and John Bowden, "Integration Of Mathematics/Numeric Analysis With Chemistry/Chemical Engineering", Retrieved on 6 December 2005 from [http://www.math.chalmers.se/stig/papers/JEE % 20paper% 20031101.pdf](http://www.math.chalmers.se/stig/papers/JEE%20paper%20031101.pdf), 2005.
- [19]. Jeffrey C. Kantor, Thomas F. Edgar, "Computing Skills In The Chemical Engineering Curriculum", *Computers in ChE*, CACHE, Corp., pp.9-56, 1996
- [20]. Damian Schofield, "Mass Effect: A Chemical Engineering Education Application Of Virtual Reality Simulator Technology", *Merlot Journal Of Online Learning And Teaching*, Vol. 8, No. 1, pp.63-75, March 2012.
- [21]. Kelvin W.W. Wong, John P. Barford, "Teaching Excel VBA As A Problem Solving Tool For Chemical Engineering Core Courses", *Chemical & Biomolecular Engineering*, Hkust, Hong Kong, Doi: [Http:// Dx.Doi.Org /10.1016/J.Ece.2010.07.002](http://dx.doi.org/10.1016/j.cbe.2010.07.002), Vol. 5, No. 4, pp. E72–E77, December 2010.
- [22]. David D. Kumar, "Computer Applications In Balancing Chemical Equations", *Journal Of Science Education And Technology*, Vol.10, No.4, pp.347-350, December 2001.
- [23]. Adilson Jose De Assis, Luis C. Oliveira-Lopes, "Free Software For Chemical Engineer's Educational Needs", 2nd Mercosur Congress On Chemical Engineering 4th Mercosur Congress On Process Systems Engineering, pp.1-11, 2006.
- [24]. Michael B. Cutlip, Mordechai Shacham, "Recent Advances In Chemical Engineering Problem Solving", *Workshop - Mathematical Software Packages*, 1, pp.1-7, 2007.
- [25]. M.R.Manafov, "Development Of A Software Application For Solving Of Problems Of Chemical Kinetics And Its Implementation In A C", *International Journal Of Engineering And Applied Sciences*, Vol.2, No.10, pp.33-37, October 2015.
- [26]. Michael B. Cutlip and Mordechai Shacham, "Integration Of Numerical Problem Solving Into The Chemical Engineering Curriculum", *Proceedings Of The 2003 American Society For Engineering Education Annual Conference & Exposition* Copyright © 2003, American Society For Engineering Education, pp.1-5, 2003.