Computational Chemical Engineering

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ABSTRACT: *Numerical methods are used for solving mathematical problems that cannot be solved analytically. Computational chemical engineering uses modern numerical analysis tools for solving differential equation models which arise in chemical engineering. These tools allow us to design, operate, and optimize the chemical production of industrial and consumer goods. This paper provides a brief introduction to computational chemical engineering.*

KEYWORDS: *computational chemical engineering, computational methods in engineering, numerical methods in chemical engineering, computer-aided chemical engineering*

I. INTRODUCTION

Chemical engineering is an engineering discipline that combines and applies the natural and life sciences with mathematics to understand and optimize the proper usage of chemicals and energy for chemical and material production. A typical chemical engineer working on a project is generally not interested in sophisticated mathematical treatments, but rather in the physical insight that he can gain from the solution of a practical and often approximate model of the chemical process being examined. A new and important tool in this regard is computational modeling, which allows quick survey calculations instead of experimentation using extremely expensive equipment and reagents [1]. Computational modeling is a cost-effective means for initial design or understanding of the behavior of chemical plants. It is not a substitute for experimentation; however, it can be effectively used to rapidly investigate numerous scenarios under different operating conditions from which an optimized set of experiments can be rationally developed. The best approach to solving most chemical engineering problems involves a judicious combination of computational modeling and experiments [2]. Chemical engineering problems can be characterized into two broad areas [3]: (1) the scope of the chemical engineering problem (chemical properties, basic chemical reactions, unit operations and unit processes, to semi-works and chemical factories), (2) inherent characteristics of the system which are defined by variables such as input materials and energy, operating conditions, and output material and energy.

II. BACKGROUND

Several problems in chemical engineering can be formulated in terms of ordinary differential equations (ODEs) or partial differential equations (PDEs). A differential equation may be regarded as an equation involving a relation between an unknown function and one or more of its derivatives. For example, one common problem encountered in engineering is the initial value problem (IVP): how does the unknown function vary with time, given some starting conditions, when is it governed by an ODE? Such ODE problems can readily be solved by MATLAB solvers.

Computational methods in chemical engineering are modern tools for solving differential equation models which arise in chemical engineering. The field embraces a wide range of problems from quantum mechanical to computer aided simulation of industrial processes. The tools used in this field include optimization, statistics, numerical analysis, mathematical modeling, operations research, simulations, and software engineering. Using the tools may require the understanding and proper use of software packages such as MATLAB, MAPLE, and MATHEMATICA. In specialized situations, it may also require being able to use programming languages such as C++ and Java.

Computational chemical engineering allows us to design, operate, and optimize the chemical production of industrial and consumer goods. It puts us in a good position to meet a broader scope of applications and situations which demand green production techniques and sustainable development [4]. Computer aids are employed at every stage from conception through design to operation. For example, chemical engineers may employ up to 200 different computer programs to aid the design and operation of efficient, nonpolluting chemical processes [5].

III. COMPUTATIONAL METHODS

There are four common numerical techniques used in chemical engineering [6,7]:

- **Finite Difference Method:** This involves the simple discretization of the ODE or PDE and replacing them with their finite difference equivalent. These finite difference approximations are algebraic in form. The difference equations are solved subject to the prescribed boundary conditions and/or initial conditions. Although the finite different method is efficient, it has difficulties with complex geometries.

- **Finite Element Method:** This is a computational technique that divides solution region into non-overlapping meshes, typically triangles in two dimensions and tetrahedral in three dimensions. It is more powerful than finite different methods in handling problems involving complex, inhomogeneous media. The systematic generality of the method makes it possible to develop a general-purpose computer programs for solving a wide variety of problems.

- **Monte Carlo Methods:** Monte Carlo methods are a set of numerical techniques that can be used to simulate the behavior of a given physical system. They are nondeterministic and are different from deterministic methods such as finite difference and finite element. They can be applied in two ways: simulation and sampling. Simulation refers to the procedure of providing mathematical imitation of real-life random phenomena. Sampling refers to methods of deducing properties of a large set of elements by studying a small, random subset.

- **Method of lines:** This technique involves discretizing a given differential equation in one or two dimensions while using analytical solution in the remaining direction. It is regarded as a special finite difference method since it combines finite different method and analytical method. It is computational efficient, numerically stable, and involves less computational time since only a small of discretization is needed.

In addition to these methods, there are hybrid methods which combine standard methods and integral transform techniques such as the Laplace transform which finds utility in solving linear ODE’s.

IV. CONCLUSION

Chemical engineers are taught to analyze problems as quantitatively as possible by using underlying basic chemical and physical principles. They are also taught to use computational methods to solve mathematical problems that cannot be solved analytically. Because computational tools are becoming an integral part to chemical engineering research, chemical engineering education should reflect this. Employers are increasingly requiring that graduates have computing skills. It is prudent and imperative that students in the modern undergraduate curriculum become used to performing basic calculations and modeling using computational software packages. However, they should keep in mind that their use of those packages does not reduce their responsibility. For more information on computational chemical engineering, one should consult several books [7-12] on the subject and other books available on Amazon.com. One should also consult the flagship journal in the field: Computers & Chemical Engineering and Journal of Computational Engineering.

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