A Step by Step Approach to the Modeling of Chemical Engineering Processes

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Using Excel for Simulation

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“To Natassia, Alessandra and Jayme”

Preface

The aim of this book is to present the issue of modeling and simulation of chemical engineering processes in a simple, didactic, and friendly way. In order to reach this goal, it was decided to write a book with few pages, simple language, and many illustrations. Sometimes, the rigor of the mathematical nomenclature has been a little simplified or relaxed, to not lose focus on the modeling and simulation. The idea was not to scare readers but to motivate them, making them feel confident and sure they are able to learn how to model and simulate even complex chemical engineering problems. The book is split into two parts: the first one (Chaps. 2, 3, and 4) deals with modeling, and the second (Chaps. 5, 6, and 7) deals with simulation.

To simplify the understanding of how to develop mathematical models, a "recipe" is proposed, which shows how to build a mathematical model step by step. This procedure is applied throughout the entire book, from simpler to more complex problems, progressively increasing the degree of complexity. For each concept of chemical engineering added to the system being modeled (kinetics, reactors, transport phenomena, etc.), a very simple explanation is given about its physical meaning to make the book understandable to students at the start of a chemical engineering course, to students of correlated areas, and even to engineers who have been away from academia for a long time.

The second part of this book is dedicated to simulation, in which mathematical models obtained from the modeling are numerically solved. There are many numerical methods available in the literature for solving the same equations. The focus of this book is not to present all of the existing methods, which can be found in excellent books about numerical methods. In this book, a few effective alternatives are chosen and applied in several practical examples. For each case, the numerical resolution is presented in detail, up to obtaining the final results. The idea is to avoid the reader getting lost in many alternatives of numerical methods, and to focus on how exactly to implement the simulation to obtain the desired results.

When using numerical methods, the simulation step can involve computational packages and programming languages. There are several computational tools for simulation, and it is not possible to say that one is better than another; however, since in most cases a chemical engineering student will work in chemical industries, this book adopts the Excel tool, which is widely used and has a very friendly interface and almost no cost. To develop computational codes, the programming language Visual Basic for Applications (VBA), available in Excel itself, will be used.

It is expected that, with this book, chemical engineering students will feel motivated to solve different practical problems related to chemical industries, knowing they can do so in an easy and fast way, with no need for expensive software.

Campinas, Brazil Liliane Maria Ferrareso Lona

Organization of the Book

Chapter 1 of the book gives a short introduction and shows the importance of the modeling and simulation issues for a chemical engineer. Important concepts needed to understand the book will also be presented.

Chapter 2 presents a "recipe" (a step-by-step procedure) to be followed to build models for chemical engineering systems, using a very simple problem. The same recipe is used throughout the entire book, to solve more and more complex problems.

Chapter 3 deals with lumped-parameter problems (in steady-state or transient regimes), in which the modeling generates a system of algebraic or ordinary differential equations. The chapter starts by applying the recipe seen in Chap. 2 to simple lumped-parameter problems, but as new concepts of chemical engineering are presented throughout the chapter, the complexity of the problems starts increasing, although the recipe is always followed.

Chapter 4 deals with distributed-parameter systems in steady-state and transient regimes, in which variables such as concentration and temperature change with the position. This kind of problem generates ordinary or partial differential equations. In this chapter, the complexity of examples increases little by little as they are presented, but all of them use the same recipe presented in Chap. 2. In this way, readers can easily understand how to build complex models.

Chapters 5, 6, and 7 are dedicated to numerically solving algebraic equations, ordinary differential equations, and partial differential equations, respectively. There are many different numerical methods available, but in these three chapters a few alternatives will be used because the main purpose of this book is to obtain a fast, robust, and simple way to simulate chemical engineering problems, not to study in detail the different numerical methods available in the literature. All simulations will be done using Excel spreadsheets or codes in VBA.

Chapter 5 uses the Newton–Raphson method to solve nonlinear algebraic equations and presents the concepts of inversion and multiplication of a matrix, available in Excel, to solve linear algebraic equations. Chapter 5 also presents an alternative based on the *Solver* tool available in Excel for both linear and nonlinear

algebraic equations. Chapter 6 uses Runge–Kutta methods to solve ordinary differential equations, and Chap. 7 adopts the finite difference method to solve partial differential equations.

I hope this book will be understandable to many people and can motivate all who wish to learn the art of modeling and simulating chemical engineering processes. Good reading!

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About the Author

Liliane Maria Ferrareso Lona received her bachelor's (1991), master's (1994), and PhD (1996) degrees in chemical engineering from the University of Campinas (Unicamp). She pursued her postdoctoral studies at the Institute for Polymer Research at the University of Waterloo, Canada, from 2001 until 2002. The subject matter in her master's and PhD courses was related to modeling and simulation of petrochemical processes, while her postdoctoral studies focused on the area of modeling, simulation, and optimization of polymerization reactors. In 1996, Liliane became professor at the School of Chemical Engineering–Unicamp, and in 2010 she became full professor with a specialization in the analysis and simulation of chemical processes. Liliane Lona taught for more than 20 times an undergraduate course related to the area of this book. She supervised dozens of grade and undergraduate students in the modeling and simulation area, and many of these works received awards, such as (i) the BRASKEM/Brazilian Association of Chemical Engineering Award (2007), (ii) the Petrobras Award Pipeline Technology (2000 and 2003), and (iii) the Regional Council of Chemistry Award (2000). Liliane published many scientific papers in reputed journals and also served as postgraduate coordinator (2006–2010) and director (2010–2014) of the School of Chemical Engineering–Unicamp.