# 1

# INTRODUCTION

Computers have revolutionized the way chemical engineers design and analyze processes, whether designing large units to make polyethylene or small microreactors to detect biological agents. In fact, the engineering problems that many of you will study as undergraduates today are similar in complexity to the problems Ph.D. students solved 30 or 40 years ago. Computer programs can now solve difficult problems in a fraction of the time it used to take. Nowadays, you no longer have to write your own software programs to use computers effectively. Computer programs can do the numerical calculations for you, but you will still need to understand how to apply these programs to specific engineering challenges.

The goal of this book is to help you practice better chemical engineering. Computers are valuable tools that enable progressive, far-reaching chemical engineering. Unfortunately, computers are not as basic as CD players, where you insert a CD, push a button, and get the same result every time. Sometimes computer programs do not work properly for the parameters you have given them. Therefore, you must be careful to use them wisely.

This book will also:

(1) Illustrate the problems that you as chemical engineers may need to solve;
(2) Compare the types of computer programs you can use and illustrate which ones are best for certain applications;
(3) Describe how to check your work to ensure you have solved the problems correctly.

This book demonstrates four computer programs: Excel®, MATLAB®, Aspen Plus®, and FEMLAB®. You may have access to other programs created by other companies. While the exact details will not be the same, the steps you take will be similar.

*Introduction to Chemical Engineering Computing*, by Bruce A. Finlayson

Computer skills are invaluable, but as an engineer, you also need to understand the physical phenomena. Each chemical engineering application chapter starts with a description of the physical problem in general terms. Then those general terms are put into a mathematical context so the computer can represent them. Next, the chapter gives several examples in which such problems are solved, providing step-by-step instructions so you can follow along on your own computer. Sometimes the same problem is solved using different programs so you can see the advantages of each program. Finally, the chapters give more complicated problems your instructor may use as homework.

Examples throughout this book demonstrate how to check your work and how to learn from the answers the computer gives you. When using computers, it is always important to know if the computer has obtained the correct answer. If you follow this strategy you will have no trouble convincing your instructor, or your boss, that you have a solution every bit as reliable as an analytical solution for a problem that cannot be solved analytically:

(1) Solve the problem
(2) Validate your work
(3) Understand how you reached that answer

## ORGANIZATION

The book is organized into 11 chapters followed by six appendices, as listed in Table 1.1. Each chapter treats a type of chemical engineering phenomenon, such as process simulation or convective diffusion. The six appendices give additional details about each computer program.

As a modern chemical engineering student, many of you are computer-savvy. This book assumes that you are not a complete beginner, but have some experience with spreadsheet programs such as Excel. The chapters provide examples and step-by-step instructions for using the computer programs to solve chemical engineering problems. If necessary, you can find more detailed information about the individual programs in the Appendices.

### Algebraic Equations

Chapters 2–5 deal with chemical engineering problems that are expressed as algebraic equations – usually sets of nonlinear equations, perhaps thousands of them to be solved together. In Chapter 2 you can study equations of state that are more complicated than the perfect gas law. This is especially important because the equation of state provides the thermodynamic basis for not only volume, but also fugacity (phase equilibrium) and enthalpy (departure from ideal gas enthalpy). Chapter 3 covers vapor–liquid equilibrium, and Chapter 4 covers chemical reaction equilibrium. All these topics are combined in simple process simulation in Chapter 5. This means that you must solve many equations together. These four chapters make extensive use of programming languages in Excel and MATLAB.

### Process Simulation

Chapter 6 introduces mass transfer problems such as distillation and absorption. Chapter 7 gives a more detailed look at process simulation, where the power of process simulators

**TABLE 1.1. Computer Programs Used in Different Chapters**

| Chapters | Excel | MATLAB | Aspen Plus | FEMLAB |
|---|---|---|---|---|
| 1: Introduction | | | | |
| 2: Equations of State | | | | |
| 3: Vapor–Liquid Equilibrium | | | | |
| 4: Chemical Reaction Equilibrium | | | | |
| 5: Mass Balances with Recycle Streams | | | | |
| 6: Simulation of Mass Transfer Equipment | | | | |
| 7: Process Simulation | | | | |
| 8: Chemical Reactors | | | | |
| 9: Transport Processes in One Dimension | | | | |
| 10: Fluid Flow in Two and Three Dimensions | | | | |
| 11: Convective Diffusion Equation in Two and Three Dimensions | | | | |
| Appendix A: Hints when Using Excel | | | | |
| Appendix B: Hints when Using MATLAB® | | | | |
| Appendix C: Hints when Using Aspen Plus | | | | |
| Appendix D: Hints when Using FEMLAB | | | | |
| Appendix E: Parameter Estimation | | | | |
| Appendix F: Mathematical Methods | | | | |

like Aspen Plus really is evident. These chapters make use of commercial codes that are run by inserting data into their custom-designed interface.

### Differential Equations

Chapters 8–11 treat problems that are governed by differential equations. Chapter 8 provides methods to model chemical reactors. These are usually initial value problems, which are illustrated in Eq. (1.1).

$$u\frac{\mathrm{d}c}{\mathrm{d}z} = -kc^2, \quad c(z=0) = c_0 \tag{1.1}$$

Note that the dependent variable, $c$, is a function of only one independent variable, $z$, and that the initial value is specified. For reactors, you start at the inlet and integrate down the reactor using either MATLAB or FEMLAB.

Chapter 9 then solves transport problems in one space dimension (1D) using FEMLAB. If you consider heat transfer through a slab, one side of the slab is kept at one temperature, $T_0$, and the other side of the slab is maintained at another temperature, $T_L$. The governing equation is

$$k\frac{\mathrm{d}^2T}{\mathrm{d}x^2} = 0 \tag{1.2}$$

with boundary conditions

$$T(0) = T_0, \quad T(L) = T_L \tag{1.3}$$

The differential equation, (1.2), is an ordinary differential equation because there is only one independent variable, $x$. In this case, equations in one space dimension are boundary value problems, because the conditions are provided at two different locations. While it is also possible to solve this problem using Excel and MATLAB, it is much simpler to use FEMLAB. Transient heat transfer in one space dimension is governed by

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \tag{1.4}$$

and this problem is solved using FEMLAB, too.

Chapters 10 and 11 use FEMLAB to solve fluid flow, heat transfer, and mass transfer problems in 2D and 3D. Here again the power of the software program shows through. You get to solve real problems that go beyond the simple 1D cases in your textbook. Those 1D problems are good for learning the subject, but in real-life situations, complications often arise that can only be handled numerically. These problems are partial differential equations, because there are two or more independent variables (say $x$ and $y$). For example, the Navier–Stokes equations in Cartesian geometry and two dimensions are

$$\begin{aligned}
\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) &= -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \\
\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) &= -\frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \\
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0
\end{aligned} \tag{1.5}$$

**Appendices**

If you need more background information while solving the problems in the book, consult the appendices. Appendices A–D discuss hints, examples, and step-by-step instructions for the four computer programs demonstrated in this book. For example, Appendix A provides useful options and terminology within Excel, while Appendix B does this for MATLAB. Appendix C provides screen images from Aspen Plus, with explanations, and Appendix D does the same for FEMLAB. Appendix E demonstrates how to use Excel or MATLAB for parameter estimation, and Appendix F illustrates the mathematical methods built into each computer program. While you will not need to program the methods, you may be curious about the mathematical analysis behind the programs.

Whether you tackle one chemical engineering problem or work chapter by chapter through the book, try to enjoy yourself. You and a classmate can sit down and work together – possibly on adjacent computers – to share insights and answer each other's questions. Remember, too: go back and forth from the application chapters to the computer program appendices; build up your knowledge bit by bit. Your reward is to be a better-trained engineer, able to compete in a fast-paced global environment.