

# *Introduction to Chemical Engineering Computing*

by

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## Preface

Chemical engineering students and chemical engineers are being asked to solve problems that are increasingly complex, whether the applications are in refineries, fuel cells, microreactors, or pharmaceutical plants. Many years ago, students wrote their own programs, first in the FORTRAN programming language, then in languages like MATLAB<sup>®</sup>. With the growth in personal computers, however, software has been written that solves many problems for students, provided they use the programs correctly. Thus, the emphasis shifted from a small group of people who were interested in writing their own programs to a large group of students who will use the programs, but don't write them. In my 38 years of teaching at the University of Washington, I taught those small groups of students how to use numerical analysis to solve complicated problems. Now, I teach *all* my students how to use the computer wisely. Only a few of the students I teach are interested in the numerical analysis (to my sorrow!), but all the students know they must be able to solve difficult problems, and they need to use the computer to do that.

The goals of this book are to illustrate (a) the problems chemical engineers have to solve, (b) the type of computer programs used to solve them, and (c) how engineers check to be sure they have solved the problems correctly. This is done in the context of how contemporary students learn – minimal reading, just-in-time learning, with lots of computer usage. The programs demonstrated here are Excel, MATLAB, Aspen Plus, and FEMLAB.

When writing this book, I assumed that readers are not absolute beginner. Junior and senior chemical engineering students have had experience with spreadsheet programs like Excel, and they can easily learn on the computer when provided a direction and key ideas or phrases. In fact, many students are more computer-savvy than their instructors. However, a beginning chemical engineering student may not know the application very well and may not have gained a solid understanding of the physical phenomena behind an engineering problem. Thus, it is important to give some explanation of why students need to solve certain problems. I have drawn on my experience to give insights into the problems in this book.

My teaching philosophy is that the problems engineers are solving today are usually intractable with analytical methods, but they can be solved with the sophisticated software available today. Thus, every engineer will be solving a problem that no one knows the answer to, and it is the engineer's job to ensure that the problem is posed correctly on paper and in the computer, and it is correctly solved. Engineering students must know how to determine if the computer solved the problem correctly by validating the work done by the computer. If they can do this, they can convince their instructor – or their future boss – that they have a solution that is every bit as reliable as an analytical solution, although without the analytical form and for a problem that can't be solved analytically.

### How to use this book in teaching

This book grew out of a course I developed at the University of Washington, first in the Winter quarter, 2003. Student evaluations of the Department indicated that students wanted more help when using the computer to solve chemical engineering assignments. Although the

students took a programming course in Computer Science, they didn't feel it was relevant to their engineering studies. I proposed an elective course for juniors that would introduce them to computer programs they would use in their education. It is called *Chemical Engineering Computer Skills* and is a lecture/laboratory course. Enrollment has grown each year, and in 2005, 70% of the junior class enrolled in this course.

As currently taught, I spend one lecture describing a problem and illustrating its solution using the computer programs. Then the class adjourns to a computer classroom where the students work in pairs, with student helpers, solving the same type of problem just demonstrated in class. Finally, the students work individually on a more difficult problem, using the same techniques, for homework credit. All the homework problems have to be correct; if not, an opportunity is given to redo them. The course is taught credit/no-credit, and credit is given provided 80% of the assignments are completed correctly. There are only 10 fifty-minute lectures and 10 laboratory sessions in the 10-week quarter. Since the applications cover much of the chemical engineering field, I joke with the students, saying, "I'm teaching you the entire field in 20 hours."

This book can also be used in a longer course. Once students have solved the elementary problems, it is easy to complicate the problems with lessons and variations that instructors would like to emphasize. Examples of such problems are provided at the end of each chapter; both introductory and advanced problems are provided. Another way to use the book is to use each chapter within different courses. Once chemical reaction equilibrium has been discussed in the Thermodynamics class, for example, instructors can hold a laboratory session that teaches computer applications, using the chapter on chemical reaction equilibrium. Other chapters would be used in other courses. In this way, the students would use the book during their entire education, in course after course. The hope is, of course, that students would then be able to concentrate more on the chemical engineering principles and use the computer as a tool.

There are four programs that are featured in this book. It is possible that your school does not use all four. While the screen images may be different, the ideas and procedures are the same. Certainly the problems can be solved using other programs. In a working environment, engineers use what their company provides. Thus, engineers may use a less powerful program because it is available. The more powerful program may cost more, too. Thus, in several chapters, the same problem is solved using different programs, which lets students see first-hand that the more general purpose programs require significantly more programming in order to solve complicated problems. In my experience, when given a suite of programs, students will use the one that allows them to solve their problem fastest.

### **Acknowledgements**

In writing this book, I owe a great thanks to the students in my classes. The first year there was no written material; students said they wanted it. The second year written material was provided, but it was clear that newer programs like FEMLAB should be emphasized. Many times, a student's question identified something that I didn't know about the program either, so all those graduates of the University of Washington (classes of 2004, 2005, and 2006) deserve my thanks. Special thanks go to Barney Santiago, who taught me one of the tricks in the book,

and Franklin Lobb, an alumnus working for AspenTech who gave valuable suggestions about Aspen Plus. I also thank Jennifer Foley, a graduate student in bioengineering that learned FEMLAB from me, because she taught me in return how to use coupling variables in FEMLAB. The Department provided a challenge grant to write textbooks, funded by a gift in the memory of alumnus Maurice Richford, BS 1926. Without that challenge grant, this book would not have been written. My daughter, Christine Finlayson, improved my writing greatly by serving as a copy editor, and the clarity is due to her work; any confusion left is my responsibility. The folks at Comsol, the makers of FEMLAB, have been very helpful as FEMLAB has been developed and grown over the past few years; Johan Sundqvist and David Kan were my major contacts. Most of all, I thank my wife, Pat, for putting up with the long hours of work that such a project requires. She has always supported me and made sacrifices that enabled me to finish.

Bruce Finlayson  
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## Chapter 1. Introduction

Computers have revolutionized the way chemical engineers design and analyze processes, whether designing large units to make polyethylene or small microreactors used to detect biological agents. In fact, the engineering problems that many of you will study as undergraduates are similar in complexity to problems PhD 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'll 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. Computer 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. Thus, you must be careful to use them wisely.

This book will also:

- (a) Illustrate the problems that you as chemical engineers may need to solve;
- (b) Compare the types of computer programs you can use and illustrate which ones are best for certain applications;
- (c) 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 won't be the same, the steps you take will be similar.

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 problems.

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's always important to know if the computer obtained the correct answer. If you follow this strategy:

- **Solve the problem**
- **Validate your work**
- **Understand how you reached that answer**

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 can't be solved analytically.

## Organization

The book is organized into eleven 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 needed, you can find more detailed information about the individual programs in the Appendices.

	Chapters	Excel	MATLAB	Aspen Plus	FEMLAB
1	Introduction				
2	Equations of State	√	√	√	
3	Vapor-liquid Equilibria	√	√	√	
4	Chemical Reaction Equilibria	√	√	√	
5	Mass Balances with Recycle Streams	√			
6	Simulation of Mass Transfer Equipment			√	
7	Process Simulation			√	
8	Chemical Reactors		√		√
9	Transport Processes in 1D				√
10	Navier-Stokes Equation in 2D and 3D				√
11	Convective Diffusion Equation in 2D and 3D				√
A	Hints when using Excel	√			
B	Hints when using MATLAB		√		
C	Hints when using Aspen Plus			√	
D	Hints when using FEMLAB				√
E	Parameter Estimation	√	√		
F	Mathematical Methods	√			

**Table 1-1. Computer programs used in different chapters**

**Algebraic Equations.** Chapters 2-5 deal with chemical engineering problems that are expressed as algebraic equations – usually sets of non-linear 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 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, 9, 10, and 11 treat problems that are governed by differential equations. Chapter 8 gives methods to model chemical reactors. These are usually initial value problems, which are illustrated in Eq. (1.1).

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

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

$$k \frac{d^2T}{dx^2} = 0 \quad (1.2)$$

with boundary conditions

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

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

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

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 won't 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 others' 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.