INTRODUCTION TO CHEMICAL ENGINEERING COMPUTING

Second Edition

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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 such as MATLAB®. However, with the growth in personal computers, 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 do not write them. In my 42 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* the 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 Comsol Multiphysics®.

When writing this book, I assumed that readers are not absolute beginners. Junior and senior chemical engineering students have had experience with spreadsheet programs such as 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 beginner chemical engineering student may not know the application very well and may not have gained a solid understanding of the physical phenomenon behind an engineering problem. Furthermore, they may not have solved very difficult problems. Thus, it is important to give some explanation of why students need to solve certain problems

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and how to overcome the obstacles when the problems tax the numerical methods. 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 cannot be solved analytically. In fact, 98% of the problems in this book are nonlinear and only a few of them have analytical solutions.

HOW TO USE THIS BOOK IN TEACHING

This book grew out of a course I developed at the University of Washington, beginning in 2003. The course is part lecture and part hands-on computer work in a computer laboratory. I usually provide simple problems for the students to solve in the laboratory, when help is available, to help them get over the barrier of using an unfamiliar program. But then, students have to solve a problem that expands their knowledge of chemical engineering and demonstrates they have used the program correctly (and described the checks they made). 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." Although I retired from teaching the course in 2009, the same objectives still apply.

This book can also be used in other courses since each chapter is keyed to a course in the curriculum. 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. The material on choice of thermodynamic model (and comparisons) also adds a bit of realism to the Thermodynamics course. Other chapters could be used in other courses. In this way, the students would use the book during their entire education, in course after course: Mass and Energy Balances, Transport of Heat, Mass, and Momentum, Reactor Design, and courses concentrating on projects such as biomedical engineering. 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. Although 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 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. The program Comsol Multiphysics comes in many modules. Nearly all the problems in this book can be solved by the basic module, although there are cases where the Chemical Reaction Engineering Module is useful. Connections with MATLAB are made with LiveLink™

for MATLAB, another module. There are only a couple of problems involving turbulent flow, and those require the CFD module. A complete list of what you get with various combinations is available from Comsol and my list is on the book website (see Appendix D).

Each chapter begins with a list of instructional objectives. In addition, the book website has a list of principles learned from each problem, both from a chemical engineering viewpoint and a computer/computer technique viewpoint. Professors that use the book are encouraged to discuss possible use in other chemical engineering courses so that more advanced problems can be solved in them, too. The indices are available on the book website, too, since students prefer using the Internet rather than turning to the back of the book; more importantly, they can be downloaded and searched for a phrase.

WHAT IS NEW?

One big change from the first edition is the fact that all four programs now have different interfaces than they did in 2005. More importantly, they have greatly enhanced capabilities. I have cut back on some explanations and refer the user to the help menus that come with the programs, since those have improved, too, and they give more information than the book can. But, I provide hints where to look.

The number of problems has approximately doubled. More importantly, the added problems are concentrated in the field of energy: integrated gas-combined cycle, including low temperature air separation, making ethanol from switchgrass, and pressure swing adsorption to make hydrogen to fuel cars. In each case a discussion of the field precedes the definition of the problem so that students can see the applicability. Microfluidics has expanded since 2005, and there are added problems in the field of biomedical applications. This has lead to many more examples and problems involving fluid flow and diffusion in two and three dimensions. An important addition was made in Aspen Plus 7.3: now you have direct access within the program to experimental data on pressure–volume–temperature of pure components and binary vapor–liquid equilibria as summarized by the National Institute of Standards and Technology. This is very important for chemical engineers, since the choice of thermodynamic model must usually be accompanied by a comparison with experimental data, and that is now made very easy—so easy that it would be unprofessional not to do the comparison. Thus, the thermodynamic sections of the book include industrial guidelines, some molecular considerations, and experimental data for comparison. Aspen Plus also has the capability to easily summarize the greenhouse impact of a process. There are talks made by professors about how they used AspenTech products in their courses; contact: University.Program@aspentech.com. One thing that is pointed out by Professor Luyben is that material and energy balances are primarily flow-based, whereas safety problems must be pressure based (and dynamic). The dynamic options are not treated here in detail, but are often covered in a control course. Aspen Plus runs under Microsoft Windows, but the author ran it under Windows by using Parallels Desktop for Mac on an Apple computer. The second edition also has examples running Aspen Plus with a simple user-defined FORTRAN program.

Some professors like to have more numerical programming in their courses, so a number of problems like that have been added to the end of many chapters. They make a good contrast—solve them using the numerical programming and then solve them using one of the four programs emphasized here to compare the ease of use of each method. Appendix E provides more detail about the numerical methods. While the programs make the numerical analysis easy to use, it is also important to recognize that most problems involve an approximation from continuous to discrete variables. A few problems in the book ask the students to do the actual numerical analysis (and compare with other programs). Instructors may say, "If you don't program the method, you haven't really understood the problem." I reply by pointing out that when a doctor prescribes an MRI, you do not say you would not do it until he/she explains how the magnetic field works in the machine, discusses hydrogen molecules flipping orientation, and describes how the imaging takes place. The doctor and technician know how to interpret the results and how to detect if the machine is not operating correctly; engineering students can do that, too.

The number of problems has been doubled, and they are organized into easy problems (subscript 1), harder problems (subscript 2), and problems that are suitable as projects, either for one student or for teams. Finally, more techniques that are in Comsol Multiphysics are explained.

The code used to solve the examples in the book is not provided on the book website, because the author believes that learning takes place when you try to duplicate the steps in the book. However, some material needed to start problems is on the book website, such as geometries for three dimensional flow/diffusion problems. Depending upon the memory of your computer, and what can be allocated to Comsol Multiphysics, some of the three dimensional problems may not be soluble on your computer. The book website is http://www.ChemEComp.com.

ACKNOWLEDGMENTS

In writing this book, I owe a great thanks to the students in my classes. Sometimes students taught me how to use an advanced technique, and their questions brought out the best of the programs. I had over 100 undergraduate research students work with me over the past decade, and the results of their work are available on my websites: http://faculty.washington.edu/finlayso/ and http://courses.washington.edu/microflo. 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, the first edition would not have been written so it could not have been revised. My daughter, Christine Finlayson, improved my writing greatly by serving as a copy editor of the first edition, and the clarity is due to her work; any confusion left is my responsibility. I thank especially Professor Stanley Sandler, University of Delaware, for reviewing the revised treatment of thermodynamics—I learned a lot, too! The folks at Comsol and Aspen Tech have been very helpful since both Comsol Multiphysics and Aspen Plus have been improved over the past few years. 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. And I was smart enough to take a few weeks off from this rewrite to celebrate our 50th wedding anniversary!

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