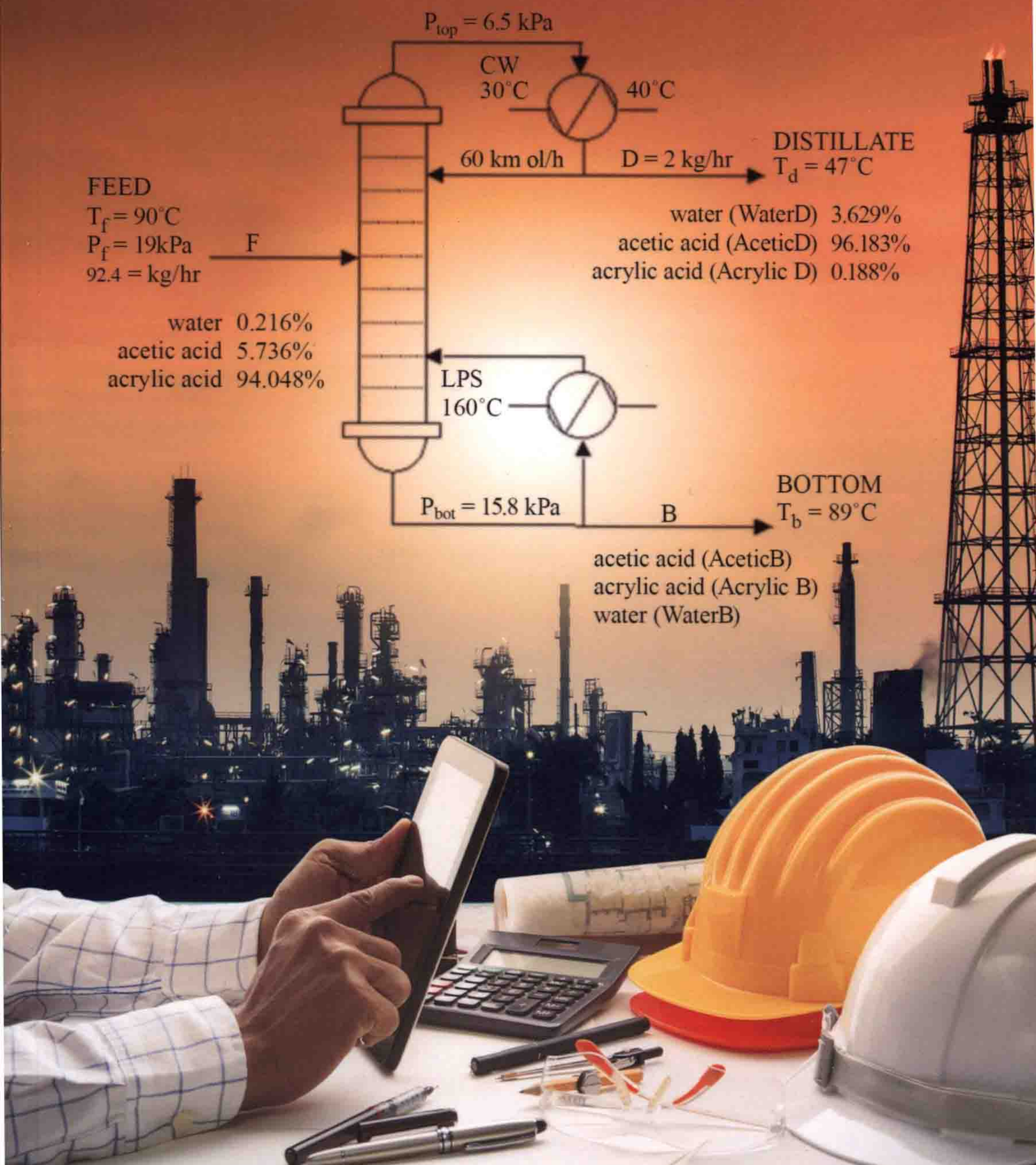
Chemical Engineering Primer with Computer Applications



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Preface

It has been observed that most of the textbooks written for introductory courses in chemical engineering follow a formal classical method. This applies, in particular, to texts for sophomore courses. Authors normally focus on writing many chapters on material balance and energy balance followed by those on allied topics. What we have used here is a different approach to offer an introductory course in chemical engineering, with emphasis on handling computer solutions for chemical engineering problems. Our aim is to introduce the reader to chemical engineering fundamentals without the distractions, which is the case with the material found in many textbooks.

This book has been written as a *beginning* chemical engineering text with emphasis on *computer applications.* The word *beginning* is the underlying paradigm of writing this book. It is the act or *process of bringing* this knowledge to young students majoring in chemical engineering at different levels. The meaning may also infer the *beginning to walk into the real world* right after finishing the bachelor's degree. In this way, this book should be of use to both chemical engineering students as a point of departure for their entry into industry and the practicing engineer for their continuing education program.

For a practicing chemical engineer, whether in industry or teaching, this book would be a good companion that adequately treats chemical engineering as a composite and integrated field.

This book covers the core concepts of chemical engineering, ranging from conservation laws all the way up to chemical kinetics. For nonengineers, who are expected to work with chemical engineers on projects, scale-ups, and process evaluations, this *primer* would be an excellent source for a solid understanding of basic concepts of chemical engineering analysis, design, and calculations.

The text is divided into three sections.

SECTION I: INSIGHT INTO CHEMICAL ENGINEERING—CHAPTERS 1 AND 2

Chapter 1, "Introductory Concepts," introduces the essentials of chemical engineering along with unit system. Chapter 2, "Basic Principles and Introduction to Calculations," reviews well-known physical and chemical laws in continuation to Chapter 1. In addition, the principles underlying chemical engineering problems are presented.

SECTION II: FUNDAMENTALS AND PROBLEM-SOLVING PROFILE—CHAPTERS 3 AND 4

This section deals with the methodology of how to devise and evaluate numerical techniques for employing computers, through standard algorithm, in order to solve chemical engineering problems. The focus of numerical methods as presented is to translate chemical engineering problems into algorithms and implement them in a spreadsheet or programming language (e.g., MATLAB®).

Chapter 3, "Numerical Methods and Chemical Engineering Computations," is devoted to introducing numerical methods with emphasis on elementary ones. Chapter 4, "The Approach to Solve Problems by Computers," illustrates how to tackle a solution of a problem by model building.

SECTION III: BACKBONE MATERIALS OF CHEMICAL ENGINEERING—CHAPTERS 5 THROUGH 10

Section III extensively covers the basic principles underlying chemical engineering in all major processes, focusing on their scientific realization and applications. Solving problems arising in fluid mechanics, distillation, chemical reaction engineering, and others is heavily emphasized in this section. The contents of the chapters are as follows:

- Chapter 5—"Fluid Flow and Transport of Fluids"
- Chapter 6—"Heat Transmission"
- Chapter 7—"Two-Phase Diffusional Operations: Distillation and Absorption"
- Chapter 8—"Reaction Kinetics, Reactor Design, and Thermodynamics"
- Chapter 9—"Process Economics and Chemical Plant Design"
- Chapter 10—"Case Studies"

The material in each chapter in Section III, excluding Chapter 10, encompasses two sections: one covers the theoretical principles in a condensed format, and the other presents a set of numerically solved problems using interactive numerical software packages.

Chapter 10, on the other hand, introduces a number of case studies that handle practical technical problems. Many of these case studies are compiled by the author in the field of applied research, in both academy and industry.

This primer in chemical engineering would serve as a text for students majoring in chemical engineering, applied chemistry, and biochemical process engineering.

This book is designed to be used by students in a variety of ways, dependent on the level of enrollment. Possible recommendations are as follows:

- Level one, sophomore students studying a course on the basic principles in chemical engineering with programming and computer applications: Chapters 1 through 4.
- Level two, junior students seeking courses on numerical solution of chemical engineering problems or/and unit operations on fluid flow and heat transfer: Chapters 1 through 6.
- Level three, senior students: The text in Chapters 7 through 9 is recommended for a course as a continuation for unit operations to cover distillation and absorption. Kinetics and reactor design and plant design are other topics to be considered for additional course(s).

This book takes a highly pragmatic approach to presenting the principles and applications of chemical engineering and offering a valuable, easily accessible guide to solve problems using computers. MATLAB and spreadsheeting are applied in solving many examples.

Problems assigned for each chapter and found in Appendix A, ranging from simple to difficult, allow readers to gradually build their skills and be able to tackle a broad range of problems in chemical engineering. In addition, the numerous real examples throughout this book (more than 70) include computer or hand solutions, or in many cases both. Many solved example problems reinforce the concepts covered. The text is written with a view that solving problems is an essential part of the learning process. It gives a taste of the kinds of problems with which chemical engineers grapple. It puts a wealth of solved practical problems at your fingertips.

One of the main unique features of this book is that it is a convenient source in chemical engineering that can be used at ease, without the need for many comprehensive texts. It is an integrated form of a *single source*.

In conclusion, one can say that two things are important: "Science…means unresting endeavor and continually progressing development toward an aim which the poetic intuition may apprehend, but the intellect can never fully grasp." Chemical engineering is the discipline that uses a molecular understanding of matter to produce—from raw materials—all the synthetic materials humankind is using.

Acknowledgments

When authors like me get involved in writing a book, they are rather being optimistic.

Optimism is the essential ingredient for success. Getting help and support from many individuals provides inspiration that fuels the author's journey through the writing process.

In this respect, I gratefully acknowledge my indebtedness to a number of colleagues who enriched this book by their valuable contributions, either in reviewing and shaping some chapters or providing sets of solved examples and problems. Helpful suggestions offered by many of them are acknowledged. On the top of the list are Dr. Adnan Zahed (KAU, Jeddah, Saudi Arabia), for his contribution to writing Chapter 6; Dr. Mazen Al-Shalbi (KFUPM, Dhahran, Saudi Arabia), for his contribution to writing Chapter 8; and Dr. Maha Abdel-Kereem and Dr. Khaled Zohdi (both with HTI, Tenth of Ramadan, and Egypt).

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Professor Abdel-Aal conducted and coordinated projects involving a wide range of process development, feasibility studies, industrial research problems, and continuing education programs for many organizations, including Suez Oil Processing Company, Petromin in Riyadh (Saudi Arabia), Arab Petroleum Investment Corp in Dhahran (Saudi Arabia), Hagler-Baily & Company, Washington DC, Mobil/Esso Oil Companies in Libya, and Kuwait oil companies.

Professor Abdel-Aal has contributed to more than 90 technical papers, is the editor of *Petroleum Economics & Engineering*, third edition (2014), and is the main author of the textbook *Petroleum and Gas Field Processing*, second edition, (2016). Both books were published by Taylor & Francis Group/CRC Press.

Professor Abdel-Aal is listed in *Who's Who in the World* (1982) and is a member of AICHE, Sigma Si, Phi Lambda Upsilon. He is a fellow and founding member of the board of directors of the International Association of Hydrogen Energy.

Introduction: Initial Thoughts

I.1 OBJECTIVES

For a student, taking the first course in their major is an exciting but scary step into the unknown. Effectively introducing chemical engineering education to undergraduate students is usually difficult, especially when teaching introductory courses. A prime pitfall of the larger texts is that students are disinclined to read several pages of text to solve a problem.

Experience in teaching the first course has shown that there is a need for such a handy, collective, and summarized source of basic principles in chemical engineering, especially when solving problems. The methodology of solving problems and their solutions should be presented hand in hand with the fundamentals, as discussed in this text.

This primer is to be considered a survival companion for students of chemical engineering. As you navigate through the text, you can maneuver smoothly from chapter to chapter. The two main themes embodied in this text are as follows:

- *Theme No. 1*: To provide students with some guide steps on how to identify the type of problems to solve and how to target a solution. Focus will be on the use of systematic algorithms that employ numerical methods to solve different chemical engineering problems by describing and transforming the information.
- *Theme No. 2*: To present the basic principles and techniques in chemical engineering and the underlying unit operations and chemical processes in a concise and nontraditional format with numerous applications.

Let us first acquaint our readers with the field of chemical engineering. All engineers employ mathematics, physics, and the engineering art to overcome technical problems safely and economically. Yet it is the chemical engineer alone that draws upon the vast and powerful science of chemistry to solve a wide range of problems. Chemical engineers use chemistry and engineering to turn raw materials into usable products, such as petrochemicals, plastics, and pharmaceutical ingredients. They apply physical science together with mathematics and computers to processes that involve physical changes and/or chemical reactions in order to produce more valuable products.

Every scientific discipline, including chemical engineering, relies on the use of computers and software. The capabilities provided by computers, such as fast calculations, large storage capacity, and software, permit engineers to solve different problems.

Therefore, scientists depend on computational methodology in solving their problems. It is based on the following fact:

> Computational science is a function of two components: theoretical and practical one.

The *theoretical* component involves the use of *systematic algorithms* to solve different scientific problems by describing and transforming the information, while the *practical* component involves the implementation of the *computational hardware and software*.

Traditionally, in solving scientific problems, researchers use either of the following:

- Theoretical approach
- Laboratory experiment

In the theoretical approach, scientists rely upon the use of some classified *models*, in accordance with how they are derived. In general, three models are well known:

1. Theoretical models (*transparent models*): These are developed using the principles of chemistry and physics.
2. Empirical models (*black box models*): These are obtained from a mathematical or statistical process of operating data—*process identification*.
3. Semiempirical models (*gray box models*): These models represent a compromise between (1) and (2), with one or more parameters to be evaluated from plant data.

Computational science, on the other hand, is different from these two traditional approaches, the theoretical and the practical, as illustrated in Figure I.1. The scientific

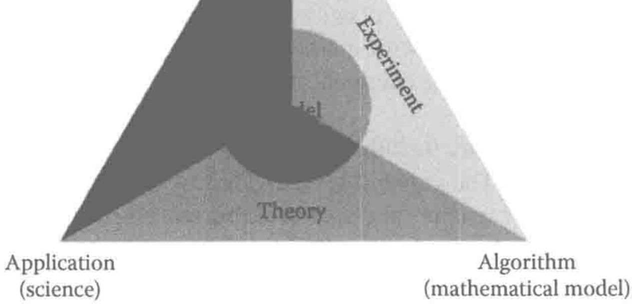

FIGURE I.1 Model of relationship among theory, computation, and experiment.

computing avenue is to gain understanding, mainly through *the analysis of mathematical models implemented on computers.*

Computers play a vital role in almost every aspect of modern chemical engineering, which may include the following applications:

1. Supercomputers to simulate complex chemical processes and plant operations
2. Computational fluid dynamics to simulate flow systems and heat transfer problems
3. MATLAB®, polymath, spreadsheeting, and others to solve many problems including differential equations
4. Aspen computer technology to simulate unit operations and processes

I.2 PROPOSED APPROACH

It was observed that frequently students had to supplement their technical knowledge when solving a problem. For example, in solving problems on flash distillation, a refresher to some basic concepts is necessary. Definitions of bubble point, dew point, and derivation of the flash equation are needed in problem solving. This book, a self-contained source on chemical engineering, will come in handy in such situations.

As an instructor in your first course, an attractive way to introduce your students to the field of chemical engineering is to present to them the following simple illustrative example of a petroleum fractionation process.

I.2.1 Illustrative Example of Petroleum Fractionation Process

Crude oil is to be fractionated into straight-run products such as gasoline and gas oil. It is heated first by heat exchangers and then desalted. Its temperature is raised next using fire heaters, before it is introduced to the fractionation tower. This process is illustrated in Figure I.2.

The next step is to explain to them how and why the crude oil is separated into products.

Well, in the transformation of raw materials (crude oil) and in the presence of energy (heat) to produce finished products, *three modes of transfer* are encountered.

Now, it may prove beneficial to examine in some detail the *transport phenomena* involved. They are known as

1. Momentum transfer (fluid flow), using a *pump*
2. Heat transfer of oil, using heat exchangers and a *furnace*
3. Mass transfer in the *distillation column* that leads to the separation of crude oil into different cuts (transfer is due to the molecular diffusion of components that separates the light from heavy)

The *physical operations* (known as unit operations and shown in the earlier example) are fluid flow, heat transfer, and distillation. They are basically based on these

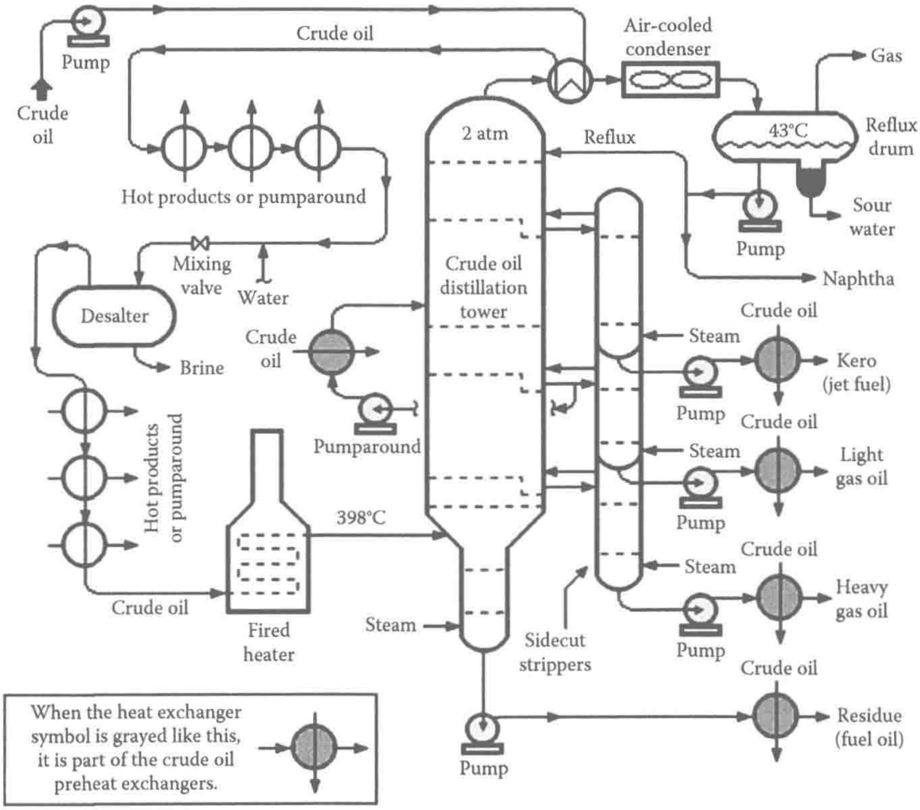

FIGURE I.2 Flow diagram for crude oil distillation.

modes of transfer. *Unit operations deal chiefly with the transfer of energy and the transfer, separation, and conditioning of materials by physical means.*

At this stage, two basic questions arise:

1. What is the mechanism(s) underlying this process?
2. How and where does it take place?

The answer to the first question deals with theory of transfer or transport, as explained, within the boundaries of our system. In answer to the second question, the combined effect of momentum, heat, and mass (MHM) is responsible for the physical changes that take place in the distillation column to produce the finished products.

Further, assume that the gasoline exiting the distillation column is introduced into what is known as a *reforming unit* in order to obtain a higher-grade gasoline. This reforming process represents a typical example of a *chemical conversion* or *chemical reaction*—known as *unit process*—where hydrocarbons undergo molecular changes and rearrangement leading to *high-octane* gasoline. *Unit processes involve primarily the conversion of materials by means of chemical reactions.* Again, it should be pointed out that the three modes of transfer, MHM, take place for operations involving chemical reactions, or chemical changes, as well.