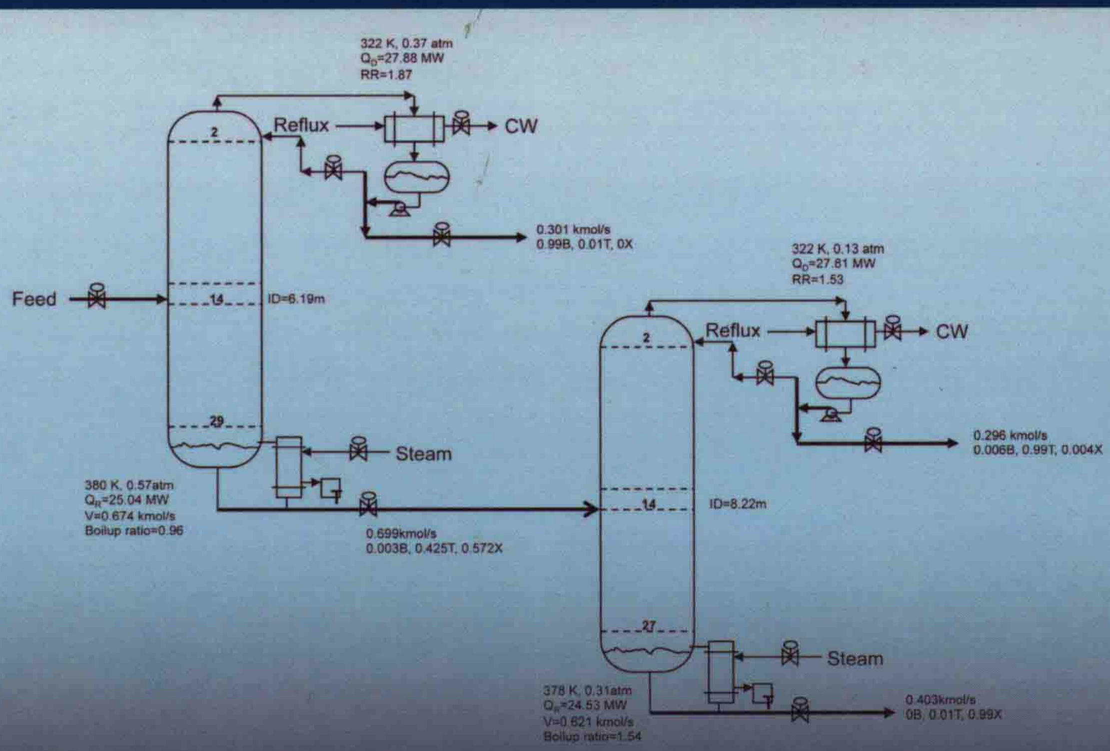
Second Edition

Distillation Design and Control Using Aspen™ Simulation

William L. Luyben



AIChE

WILEY

DISTILLATION DESIGN AND CONTROL USING ASPEN™ SIMULATION

Second Edition

WILLIAM L. LUYBEN
Lehigh University
Bethlehem, Pennsylvania

AIChE®

WILEY

Cover design: John Wiley & Sons, Inc.
Cover image: © William L. Luyben

Published by John Wiley & Sons, Inc., Hoboken, New Jersey.
Published simultaneously in Canada.

Library of Congress Cataloging-in-Publication Data

Luyben, William L.
Distillation design and control using Aspen simulation / William L Luyben. – 2nd ed.
p. cm.
"AIChE."
Includes index.
ISBN 978-1-118-41143-8 (cloth)
1. Distillation apparatus–Design and construction. 2. Chemical process control–Simulation methods. 3. Petroleum–Refining. I. American Institute of Chemical Engineers. II. Title.
TP159.D5L89 2013
660'.28425–dc23

2012030047

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

DISTILLATION DESIGN AND CONTROL USING ASPEN^{TM} SIMULATION

This book is dedicated to farmers all over the world.
No Farmers, No Food!

PREFACE TO THE SECOND EDITION

Distillation fundamentals do not change, nor does the importance of distillation in our energy-intensive society. What does change is the range of applications and methods of analysis that provide more insight and offer improvements in steady-state design and dynamic control. In the seven years since the first edition was published, a number of new concepts and applications have been developed and published in the literature.

Industrial applications of the divided-wall (Petlyuk) column have expanded, so a new chapter has been added that covers both the design and the control of these more complex coupled columns. The use of dynamic simulations to quantitatively explore the safety issues of rapid transient responses to major process upsets and failures is discussed in a new chapter. A more structured approach for selecting an appropriate control structure is outlined to help sort through the overwhelmingly large number of alternative structures. A simple distillation column has five factorial (120) alternative structures that need to be trimmed down to a workable number, so that their steady-state and dynamic performances can be compared.

Interest in carbon dioxide capture has become more widespread, so a chapter studying the design and control of the low-pressure amine absorber/stripper system and the high-pressure physical-absorption absorber/stripper system has been added. The capabilities and features in Aspen software have been updated. The importance of being able to operate columns over a wide ranges of throughputs has increased with the development of chemical plants that are coupled with power-generation processes or inherently intermittent "green" energy sources (solar and wind). A new chapter deals with column control structures that can effectively deal with these turndown issues.

I hope you find the new edition useful and understandable. The coverage is unapologetically simple and practical. Therefore, the material should have a good chance of actually being applied to real and important problems. Good luck in your distillation design and control careers. I think you will find it challenging but fun.

William L. Luyben

PREFACE TO THE FIRST EDITION

The rapid run up in the price of crude oil in recent years and the resulting "sticker shock" at the gas pump have caused the scientific and engineering communities to finally understand that it is time for some reality checks on our priorities. Energy is the real problem that the world faces, and it will not be solved by the recent fads of biotechnology or nanotechnology. Energy consumption is the main producer of carbon dioxide, so it is directly linked with the problem of global warming.

A complete reassessment of our energy supply and consumption systems is required. Our terribly inefficient use of energy in all aspects of our modern society must be halted. We waste energy in our *transportation* system with poor-mileage SUVs and inadequate railroad systems. We waste energy in our *water* systems by using energy to produce potable water, and then flush most of it down the toilet. This loads up our *waste disposal* plants, which consume more energy. We waste energy in our *food* supply system by consuming large amounts of energy for fertilizer, tillage, transporting, and packaging our food for consumer convenience. The old farmer markets provided better food at lower cost and required much less energy.

One of the most important technologies in our energy-supply system is distillation. Essentially, all our transportation fuel goes through at least one distillation column on its way from crude oil to the gasoline pump. Large distillation columns called pipestills separate the crude into various petroleum fractions based on boiling points. Intermediate fractions go directly to gasoline. Heavy fractions are catalytically or thermally "cracked" to form more gasoline. Light fractions are combined to form more gasoline. Distillation is used in all of these operations.

Even when we begin to switch to renewable sources of energy, such as biomass, the most likely transportation fuel will be methanol. The most likely process is the partial oxidation of biomass to produce synthesis gas (a mixture of hydrogen, carbon monoxide, and carbon dioxide), and the subsequent reaction of these components to produce methanol and water. Distillation to separate methanol from water is an important part of this process. Distillation is also used to produce the oxygen used in the partial oxidation reactor.

Therefore, distillation is, and will remain in the twenty-first century, the premier separation method in the chemical and petroleum industries. Its importance is unquestionable in helping to provide food, heat, shelter, clothing, and transportation in our modern society. It is involved in supplying much of our energy needs. The distillation columns in operation around the world number in the tens of thousands.

The analysis, design, operation, control, and optimization of distillation columns have been extensively studied for almost a century. Until the advent of computers, hand calculations and graphical methods were developed and widely applied in these studies. Starting from about 1950, analog and digital computer simulations began to be used for solving many engineering problems. Distillation analysis involves iterative vapor–liquid phase equilibrium calculations and tray-to-tray component balances that are ideal for digital computation.

Initially, most engineers wrote their own programs to solve both the nonlinear algebraic equations that describe the steady-state operation of a distillation column and to numerically integrate the nonlinear ordinary differential equations that describe its dynamic behavior. Many chemical and petroleum companies developed their own in-house steady-state process-simulation programs in which distillation was an important unit operation. Commercial *steady-state* simulators took over about two decades ago and now dominate the field.

Commercial *dynamic* simulators were developed quite a bit later. They had to wait for advancements in computer technology to provide the very fast computers required. The current state-of-the-art is that both steady-state and dynamic simulations of distillation columns are widely used in industry and in universities.

My own technical experience has pretty much followed this history of distillation simulation. My practical experience started back in a high-school chemistry class in which we performed batch distillations. Next came an exposure to some distillation theory and running a pilot-scale batch distillation column as an undergraduate at Penn State, learning from Arthur Rose and "Black" Mike Cannon. Then, there were five years of industrial experience in Exxon refineries as a technical service engineer on pipestills, vacuum columns, light-ends units, and alkylation units, all of which used distillation extensively.

During this period, the only use of computers that I was aware of was for solving linear programming problems associated with refinery planning and scheduling. It was not until returning to graduate school in 1960 that I personally started to use analog and digital computers. Bob Pigford taught us how to program a Bendix G12 digital computer, which used paper tape and had such limited memory that programs were severely restricted in length and memory requirements. Dave Lamb taught us analog simulation. Jack Gerster taught us distillation practice.

Next, there were four years working in the Engineering Department of DuPont on process-control problems, many of which involved distillation columns. Both analog and digital simulations were heavily used. A wealth of knowledge was available from a stable of outstanding engineers: Page Buckley, Joe Coughlin, J. B. Jones, Neal O'Brien, and Tom Keane, to mention only a few.

Finally, there have been over 35 years of teaching and research at Lehigh in which many undergraduate and graduate students have used simulations of distillation columns in isolation and in plantwide environments to learn basic distillation principles and to develop effective control structures for a variety of distillation column configurations. Both home-grown and commercial simulators have been used in graduate research and in the undergraduate senior design course.

The purpose of this book is to try to capture some of this extensive experience with distillation design and control, so that it is available to students and young engineers when they face problems with distillation columns. This book covers much more than just the mechanics of using a simulator. It uses simulation to guide in developing the optimum economic steady-state design of distillation systems, using simple and practical approaches. Then, it uses simulation to develop effective control structures for dynamic control. Questions are addressed of whether to use single-end control or dual-composition control, where to locate temperature control trays, and how excess degrees of freedom should be fixed.

There is no claim that the material is all new. The steady-state methods are discussed in most design textbooks. Most of the dynamic material is scattered around in a number of papers and books. What is claimed is that this book pulls this material together in a coordinated easily accessible way. Another unique feature is the combination of design and control of distillation columns in a single book.

There are three steps in developing a process design. The first is conceptual design in which simple approximate methods are used to develop a preliminary flowsheet. This step for distillation systems is covered very thoroughly by Doherty and Malone (*Conceptual Design of Distillation Systems*, 2001, McGraw–Hill). The next step is preliminary design in which rigorous simulation methods are used to evaluate both steady-state and dynamic performance of the proposed flowsheet. The final step is detailed design in which the hardware is specified in great detail: types of trays, number of sieve tray holes, feed and reflux piping, pumps, heat-exchanger areas, valve sizes and so on. This book deals with the second stage, preliminary design.

The subject of distillation simulation is a very broad one, which would require many volumes to cover comprehensively. The resulting encyclopedic-like books would be too formidable for a beginning engineer to try to tackle. Therefore, this book is restricted in its scope to only those aspects that I have found to be the most fundamental and the most useful. Only continuous distillation columns are considered. The area of batch distillation is very extensive and should be dealt with in another book. Only staged columns are considered. They have been successfully applied for many years. Rate-based models are fundamentally more rigorous, but they require that more parameters be known or estimated.

Only rigorous simulations are used in this book. The book by Doherty and Malone is highly recommended for a detailed coverage of approximate methods for conceptual steady-state design of distillation systems.

I hope that the reader finds this book useful and readable. It is a labor of love that is aimed at taking some of the mystery and magic out of design and operating a distillation column.

W. L. L.

CONTENTS