A LOW LATENCY ALGORITHM FOR THE SIMULATION OF A BINARY
DISTILLATION COLUMN USING A SPREADSHEET

By

Robert Bruce Coulter

Tricia A.W. Thomas
Assistant Professor
(Advisor)

Frank Jones
U.C. Foundation Professor
(Committee Member)

Bryan Ennis
Associate Professor
(Committee Member)

James W. Hiestand
U.C. Foundation Professor
(Committee Member)
A LOW LATENCY ALGORITHM FOR THE SIMULATION OF A BINARY DISTILLATION COLUMN USING A SPREADSHEET

By

Robert Bruce Coulter

A Thesis Submitted to the Faculty of the University of Tennessee at Chattanooga in Partial Fulfillment of the Requirements of the Degree of Master of Science: Engineering

The University of Tennessee at Chattanooga
Chattanooga, Tennessee

May 2015
Copyright @ 2015

By Robert Bruce Coulter

All Rights Reserved
ABSTRACT

Increases in the run speed of readily available computing resources has significantly improved the performance of distillation design and simulation algorithms. Presented here is an algorithm for the simulation of a binary distillation column with a near instantaneous response of the output variables to changes in the input variables (low latency). A discussion of the evolution of distillation analysis methods in conjunction with the improvements in computing power is included. Emphasis is on the impact of these advanced methods on the demonstration and characterization of distillation concepts. A direction for the development of fast algorithms for the modeling of multi-component distillation systems is also discussed.
ACKNOWLEDGEMENTS

I thank my advisor, Dr. Tricia Thomas, for her guidance and the committee members for their comments and suggestions for this effort. I also thank the management of Chattanooga State Community College for their support of my graduate work at UTC.
TABLE OF CONTENTS

ABSTRACT......................................................................................................................................................iv

DEDICATION....................................................................................................................................................v

ACKNOWLEDGEMENTS..............................................................................................................................vi

LIST OF TABLES..............................................................................................................................................viii

LIST OF FIGURES..........................................................................................................................................ix

LIST OF ABBREVIATIONS.............................................................................................................................x

CHAPTER

1. INTRODUCTION.............................................................................................................................................1

1.1 Background...............................................................................................................................................1

1.2 Explanation of Terms................................................................................................................................2

1.2.1 The Distillation Problem....................................................................................................................2

1.2.2 Design Versus Simulation................................................................................................................5

1.2.3 Iteration Levels....................................................................................................................................7

1.2.4 Readily Available Computing Resources.........................................................................................8

1.2.5 Ideal Versus Non-ideal.......................................................................................................................9

1.2.6 Mathematical Notations and Diagrams.............................................................................................10

1.3 Mathematical Issues of the Distillation Problem................................................................................13

1.3.1 Mathematical Issues of Non-linear Simultaneous Equations.........................................................13

1.3.2 Non-linear Equilibrium Relationships............................................................................................13

1.3.3 Growth of Iteration Levels..............................................................................................................15

2. LITERATURE REVIEW OF DISTILLATION ALGORITHMS.................................................................18

2.1 Introduction...............................................................................................................................................18

2.2 Graphical Models...................................................................................................................................19

2.2.1 McCabe-Thiele Model.....................................................................................................................19

2.2.1.1 McCabe-Thiele Introduction....................................................................................................19

2.2.1.2 McCabe-Thiele Method..........................................................................................................20

2.2.2 Ponchon-Savarit (PS) Model........................................................................................................25
LIST OF TABLES

1.1 Design and Simulation Distillation Problems.................................................................6
4.1 Ethanol / Water Vapor Equilibrium Data........................................................................56
4.2 Comparison of Single Line Azeotropic Equilibrium Model to Actual Data -
    Ethanol / Water ...........................................................................................................57
4.3 Comparison of Single Line Non-azeotropic Model to RV Model
    and Actual Data - Methanol / Water...........................................................................58
4.4 Margules Non-ideal Equilibrium Model with Temperature Estimation -
    Ethanol / Water...........................................................................................................59
LIST OF FIGURES

1.1 Distillation Column Diagram.................................................................12

2.1 McCabe-Thiele Diagram........................................................................25

2.2 Ponchon-Savarit Diagram........................................................................27

2.3 Cunningham-McGann McCabe-Thiele Spreadsheet Screenshot..................30

2.4 Wolfram MT Interactive Model...............................................................30

3.1 Top Half of Algorithm Implementation in LibreOffice Calc.....................40

3.2 Bottom Half of Algorithm Implementation in LibreOffice Calc...............41

3.3 Implementation of Algorithm on Microsoft Excel with Slider Controls.......42
LIST OF ABBREVIATIONS

BP, Bubble Point
EA, Exponential Azeotropic
ENA, Exponential Non-azeotropic
LM, Lewis – Matheson
LOC, Line of Code
MNIMTE, Margules Non-ideal Model with Temperature Estimation
MT, McCabe -Thiele
PS, Ponchon – Savrit
RACR, Readily Available Computing Resources
RCM, Rigorous Computer Methods
RV, Relative Volatility
SC, Spreadsheet Code
SR, Sum Rates
TC, Traditional Code
TG, Thiele-Geddes
VBA, Visual Basic for Applications
VLE, Vapor Liquid Equilibrium
WC, Wizard Code
CHAPTER 1
INTRODUCTION

1.1 Background

The motivation for this effort was to determine the most effective way to demonstrate distillation using current technology. A secondary motivation was to find more effective methods for the simulation and design of a distillation column using readily available computing resources (RACR).

The mathematical model of a distillation system is very complex requiring either advanced computing power, if available, or efficient algorithms in the case of limited or no computing resources. It has been noted, however, that although there have been tremendous advances in the availability and power of computing resources in the last sixty years, the incorporation of these resources into engineering textbooks is limited. It is generally presumed that these advances, for the most part, are inside proprietary software similar to Aspen (AspenTech 2015). The developers of such software, of course, have little incentive to disclose their specific algorithms to educators and students. They do, however, usually indicate the basic assumptions behind their models.

The authors of engineering textbooks have not ignored the progress of technology. Instead, it is perhaps that there has been little motivation to change the methods of modeling distillation. Maybe a reason for this is that a typical writer of engineering textbooks does not want to be distracted explaining computer coding techniques in the midst of showing distillation
concepts. Another reason may be that the typical writer for engineering textbooks does not perceive that technology offers improvement to the graphical solution of distillation problems. The goal of this paper is to show that this belief is incorrect. A spreadsheet method is shown in chapter 3 that depicts a binary distillation simulation with a wide degree of user input options. This, coupled with the impressive array of graphic displays available in spreadsheets, should make a significant advance in conveying the deep mathematical concepts of distillation.

It is hoped that the distillation modeling tools presented here will be incorporated in educational and industrial settings.

1.2 Explanation of Terms

1.2.1 The Distillation Problem

Much of this paper will frequently refer to the distillation problem. This has a specific meaning in the context of this paper and is not meant to apply to all distillation problems. The distillation problem is:

What are the unknown parameters of a steady state distillation column system that has a single saturated feed of a given flow and known composition?

In the determination of the distillation problem, the following additional assumptions are made:

1. The pressure is known and is constant throughout the column.
2. Product is removed as saturated liquid only at the bottom and top of the column.
3. There are no heat losses.

Other assumptions will be made on a case-by-case basis (particularly in regards to feed quality, enthalpy and the equilibrium relationships), but the above assumptions will always apply. Generally, depending on how the equations are written, the number of unknowns, U, for the distillation problem is:
\[ U = 2C(T+1) + 1 \]

(1.1)

\[ T = \text{Number of trays} \]
\[ C = \text{Number of components} \]

The above equation only considers \((C-1)\) unknown concentrations (mole fractions) since the last mole fraction can be trivially recovered by subtracting all known mole fractions from one. For example, in a two component (binary) system, only the concentration of one component is utilized in solving a given problem. Therefore usually no reference is given to the other component in a binary system. Note that the number of unknowns increases rapidly with the increase in trays and components.

The simplest distillation problem has no trays, \(T=0\), and two components, \(C=2\), and so has only the reboiler acting as a stage (see Fig. 1.1). This is called a flash problem and has only five unknowns:

- \(L_0\) - Bottoms flow rate
- \(D\) - Top (distillate) flow rate
- \(X_0\) - Bottoms mole fraction
- \(Y_0\) - Top (distillate) mole fraction
- \(V_0\) – Vapor Flow Rate

The five equations that resolve these five unknowns are:

\[ F = L_0 + D \]  \quad (1.2)
\[ FX_F = L_0X_0 + DY_0 \]  \quad (1.3)
\[ Y_0 = \frac{Y(X_0)}{Z} \]  \quad (1.4)
\[ D = V_0(1-R_F) \]  \quad (1.5)
\[ V_0 = \frac{Q}{\Delta H(X_0)} \]  \quad (1.6)

The variables are as follows:

- \(F\) = Feed flow rate \([\text{moles/time}]\)
- \(X_F\) = Feed mole fraction
- \(L_0\) = Bottoms flow rate \([\text{moles/time}]\)
- \(D\) = Distillate flow rate \([\text{moles/time}]\)
- \(X_0\) = Bottoms mole fraction
- \(Y_0\) = Distillate mole fraction
- \(R_F\) = Fraction of Vapor \((V_0)\) returned to column (a.k.a., reflux fraction)
\[ Q = \text{Heating rate to reboiler [Energy/time]} \]
\[ V_0 = \text{Vapor rise rate [moles/time]} \]
\[ R = \text{Reflux flow rate [moles/time]} \]

The equations represent the following:

(1.2) - Overall Material (Mole) Balance
(1.3) - Component Material Balance (C-1 equations required)
(1.4) - Equilibrium Equation (C-1 equations required)
(1.5) - Reflux Equation (For Flash problems, \( R_F \) is typically zero)
(1.6) - Energy Balance

\( \gamma \) is the equilibrium operator that maps the liquid concentration(s) to the vapor concentration(s) at equilibrium. \( \Delta H \) is the enthalpy function that maps the liquid concentration(s) to its molar heat of vaporization. Much of the difficulty in solving distillation problems involves finding suitable functions and operators -- particularly the equilibrium operator.

A slightly more complex flash problem would involve \( (C=3) \) components. In this case, Eq. (1.1) indicates seven unknowns. It is now required to have material balance and equilibrium equations for another component although we can still ignore the third component as long as the overall material balance equation Eq. (1.2) is used.

Another example to consider is adding a tray \( (T=1) \) with two components \( (C=2) \). Eq. (1.1) tells us that there are nine unknowns. The additional unknowns are:

\[ L_1 - \text{the liquid flowing off tray 1} \]
\[ V_1 - \text{the vapor leaving tray 1} \]
\[ X_1 - \text{the liquid mole fraction on tray 1} \]
\[ Y_1 - \text{the vapor mole fraction leaving tray 1} \]

The four additional equations needed to resolve all nine unknowns are two material balance equations, an energy balance equation and an equilibrium equation. All four of these equations are done only around a control boundary (bubble) surrounding the reboiler (just below the tray).

Imagine a binary distillation column with twenty trays (which would not be considered large by industry standards). For this, Eq. (1.1) indicates 85 unknowns and therefore 85
equations to resolve this system. The above examples indicate that distillation is difficult to
depict mathematically.

1.2.2 Design Versus Simulation

Within the context of distillation it is useful to divide problems into two types:

1. Design (or Engineering) problems
2. Simulation (or Operation) problems

A distillation design problem is generally concerned with finding the physical configuration and
equipment settings that produce specified output stream parameters from a specified input stream
parameters. A typical design problem might be:

What is the minimum number of distillation column trays needed to produce an overhead stream
of at least 90 mole % ethanol from a feed containing 30 mole % ethanol?

A distillation simulation problem is generally concerned with finding output stream
parameters from specified input parameters and specified operational settings. A typical
simulation problem might be:

What is the overhead stream concentration of a 20 tray column being fed at the 15th tray with 30
mole % ethanol with a vapor rise rate that is 50 % of the feed flow rate and a reflux of 70 %?

The following table gives typical known and unknown parameters of distillation design and
simulation problems:
Table 1.1

Design and Simulation Distillation Problems

<table>
<thead>
<tr>
<th>Known Parameters</th>
<th>Design</th>
<th>Simulation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1. Feed flowrate and concentration</td>
<td>1. Feed flowrate and concentration</td>
</tr>
<tr>
<td></td>
<td>2. Product flowrates and concentrations</td>
<td>2. Heat input</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3. Reflux fraction</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4. Number of trays</td>
</tr>
<tr>
<td>Unknown Parameters</td>
<td>1. Number of trays</td>
<td>1. Product flowrates and concentrations</td>
</tr>
<tr>
<td></td>
<td>2. Heat input</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3. Reflux fraction</td>
<td></td>
</tr>
</tbody>
</table>

There is no strict rule separating design problems from simulation problems. The distinction is made because of typical situations encountered in industry. If one is interested in constructing a distillation column the analysis will typically be a design problem. If one is interested in the capabilities of an existing distillation column, the analysis will typically be a simulation problem.

Another key difference between design and simulation algorithms is that simulation algorithms are often expected to be fast by either employing efficient algorithms or be deployed on high performance (most likely expensive) computing hardware. For example, a low performance flight simulator might suffer from low frame rates as one flies near buildings. Ideally, it is desired to have low latency algorithms in simulation programs. That is, one wants a fast (hopefully unnoticeable) recalculation of the output parameters whenever the user changes an input parameter.

Most of the analysis in this paper will be focused on the simulation problem because of the author's work with two distillation columns used for training purposes at the Wacker Institute, Chattanooga, TN. The operational limits of these columns were analyzed by Murat Ozkaya (Ozkaya). In the current work, algorithms were developed that allowed the simulation of these
columns on classroom computers. The motivation for this is similar to the reason that airline pilots receive much of their training on flight simulators. The simulators allow the student to gain an understanding of the capabilities and limits without incurring the costs and safety risks of actual operation.

1.2.3 Iteration Levels

Nearly all searches for solutions involve iterative (trial and error) methods. One measure of the difficulty of solving a particular distillation problem is the depth and/or number of levels of iterations required. If only one unknown parameter must be solved by iteration and all other parameters can be determined explicitly from an initial guess of that parameter, then we call that a one level or single tiered iteration (or one iteration loop) problem. A good example of this is the flash problem where the flash temperature is guessed and then all parameters checked for errors. Based on the error, the temperature can be corrected and the calculations checked again until the error is reduced to an acceptable value. Multiple loops of iteration are often encountered in multi-component \((C > 2)\) distillation problem where an iterative loop must be done for each tray. Nested iteration loops can occur in a situation when two or more parameters cannot be solved explicitly. For example, assume a system of equations which includes unknown parameters \(G\) and \(K\). A trial value is \(G\) is guessed. An iterative search for the value of \(K\) is required that corresponds to this guessed value of \(G\). In other words, the search for \(K\) is nested inside the search for \(G\). At this point all remaining parameters can be explicitly determined and checked for errors. The value of \(G\) can then be adjusted based on this error and the iteration process is repeated until an acceptable error (e.g. within 0.1 \%\) is achieved. This type of nested iteration scheme is double-tiered. Let's assume that on average ten iteration loops
are needed to find $G$, and that for every instance of $G$ tried ten iteration loops are needed to find $K$. Then the number of iteration loops for finding $K$ are $10^2 = 100$. It is quite apparent that nested iteration loops should be avoided.

### 1.2.4 Readily Available Computing Resources

The speed and accuracy of solving a particular distillation problem depends on the available computing resources. One of the goals of this paper is to delineate between those algorithms compatible with RACR and those that are not. For purposes of this paper RACR is defined as follows:

Computing resources that more than 75% of 4th year US engineering students can access and the skills to use. At the time of this writing, the author believes that this is a personal computer with installed spreadsheet software.

RACR has changed significantly in the last forty years. The author witnessed a sudden change in RACR which occurred in the mid 1970s as pocket calculators became readily available. Before the turn of the century, personal computers with popular software pre-installed became readily available.

An important point in the definition of RACR is the phrase, “skills to use”. Software installed on a personal computer does not, of course, imply the ability to use it. Distillation problems generally require programmable software. Programmable software can be divided into three categories. They are listed here from the easiest to most difficult to use:

1. **Configurable (WC)** - Employs selection windows and wizards where the user only has to make choices from a lists and enter data. The user is generally not expected to enter equations or logic statements. We will call this type of programming Wizard Code (WC). Generally, proprietary software is in this category.
2. **Spreadsheet (SC)** - Employs a grid of cells where data or a single line of code (LOC) can be entered into each cell. The output of the code is automatically displayed in the cell. The user is expected to understand the spatial logic of the interaction of cells, however, based on the design of spreadsheets, the user does not need to be concerned with chronological (temporal logic) action of the program.

3. **Traditional Coding (TC)** – Logic statements are entered sequentially. The user must be aware of spatial (memory location) logic and temporal logic (when a statement is executed). This includes programs in FORTRAN, BASIC, and PERL.

   Currently, engineering students are usually required to receive training in TC, and some type of TC software is usually installed on students' computers. It is believed, however, that this does not meet the definition of RACR because only a minority of students actually acquire the necessary skill levels to effectively employ it. The author believes that most engineering students have the skill to employ WC and SC. WC, unfortunately, is the facade of expensive proprietary software which is the reason it is not included in the RACR definition above.

   It is also believed that the teaching of engineering principles is most effective when RACR is incorporated into the learning environment.

### 1.2.5 Ideal versus Non-ideal

With regard to equilibrium equations it is convenient to refer to systems as being either ideal or non-ideal. This has very specific meaning in the field of thermodynamic vapor / liquid equilibrium. To avoid an in-depth discussion of the topic, the following equation will be assumed to apply if a system is referred to as being ideal:

\[ Y_i P = X_i P^* \]  \hspace{1cm} (1.7)
\[ Y_i = \text{Mole fraction of component } i \text{ in the vapor phase} \]
\[ P = \text{System pressure} \]
\[ X_i = \text{Mole fraction of component } i \text{ in the liquid phase} \]
\[ P_i^* = \text{Vapor pressure of pure } i \text{ at the system temperature} \]

The above equation assumes that the ideal gas law applies to the vapor phase, and that the liquid phase forms an ideal mixture.

The following equation will be assumed to apply if the system is referred to being non-ideal in this paper:

\[ Y_i P = \gamma_i X_i P_i^* \quad (1.8) \]

\[ Y_i = \text{Mole fraction of component } i \text{ in the vapor phase} \]
\[ P = \text{System pressure} \]
\[ X_i = \text{Mole fraction of component } i \text{ in the liquid phase} \]
\[ P_i^* = \text{Vapor pressure of pure } i \text{ at the system temperature} \]
\[ \gamma_i = \text{Activity coefficient of component } i \]

The above equation still assumes that the vapor phase can be represented with the ideal gas law. This is generally a safe assumption as long as the system being analyzed operates at low to moderate pressures and under non-cryogenic conditions. This is usually the case for most distillation systems, but one should be aware that Eq. (1.8) cannot be universally applied to all non-ideal distillation systems.

### 1.2.6 Mathematical Notation and Diagrams

To reflect their use in spreadsheets, the following mathematical notation is sometimes used:

* means multiplication
^ means exponentiation

Expressions like \( Y(X), T(X), \text{ and } H(X) \) are functions of \( X \) (not products). Functions (or operators) are indicated with an underline.
The subscript for a liquid or vapor mole fraction (e.g. $X_2$, $Y_2$) may refer to a particular component, tray number, location or a particular data point. Generally, when referring to distillation problems, the subscripts represent tray numbers or locations. When discussing the development of equilibrium equations, the subscripts generally refer to a particular component and/or data point (e.g. from VLE data). For binary systems, sometimes the subscript index $l$ is dropped for convenience (e.g. $X_l = X$).
Figure 1.1 Distillation Column Diagram
1.3 Mathematical Issues of the Distillation Problem

1.3.1 Mathematical Issues of Non-linear Simultaneous Equations

The distillation problem can be represented by simultaneous equations (determined from the material, energy balances and equilibrium relationships) with the following convenient form as shown by Charles Broyden (Broyden 1965):

\[
\begin{align*}
    f_1(z_1, z_2, \ldots, z_n) &= 0 \\
    f_2(z_1, z_2, \ldots, z_n) &= 0 \\
    \vdots \\
    f_n(z_1, z_2, \ldots, z_n) &= 0
\end{align*}
\]  \quad (1.9)

If the above set of equations are all linear, they can be easily solved by many standard methods from linear algebra – e.g. Gaussian Reduction. Unfortunately, the equilibrium relationships in the distillation problem involve non-linear terms, which in nearly all cases, will require an iterative search for the unknowns. Broyden describes some of these methods, however, as he points out, these methods are not always reliable. Part of the difficulty is the reliance on obtaining accurate estimates of the partial derivatives of \( f_n \). Also, if the initial guesses for the unknowns are not sufficiently close, the algorithm may diverge away from the solution. More details on Broyden's method as applied to multi-component distillation are discussed by Komissarov (Komissarov and Sang 2014).

1.3.2 Non-linear Equilibrium Relationships

Another difficulty embedded in the system (1.9) is that the equilibrium relationships are difficult to mathematically model in themselves. The equilibrium models are also difficult to verify. To illustrate, let's imagine the perfect error-free non-linear operator, \( Y_P \), that represents the equilibrium relationships that are embedded in the system of equations (1.9). It is known that \( Y_P \) is set by the components in the distillation system. This can be represented as:
\[(C_1, C_2, C_3 \ldots) \rightarrow Y_P \quad (1.10)\]

\(C_1, C_2, C_3 \ldots\) represent the components in the system. It is assumed that only chemical property data are available for each component and is available (no mixture data). Unfortunately, it is not currently possible to determine \(Y_P\) in this manner. Instead one looks for approximations of \(Y_P\). This can be imagined by the following sequence:

\[Y_A, Y_B, Y_C \ldots \rightarrow Y_P \quad (1.11)\]

As the index increases the complexity of the non-linear operator increases. The improvement in accuracy, however, is not easily determined. In other words, it is not easy to quantify the improvement in accuracy achieved by pursuing a more complex (and presumably more accurate) operator. For example, suppose \(Y_A\) is the operator determined by assuming that the distillation system components are ideal (see 1.2.5). One can then, with more effort, determine \(Y_B\) which will be assumed to be the Margules activity coefficient model (Perry and Green 1997, p. 13-21). If the data generated from using \(Y_A\) and the data generated from \(Y_B\) are sufficiently close (e.g. within 5\%), then one might be more confident about using either \(Y_A\) or \(Y_B\). Alternatively, if the data generated from using \(Y_A\) and the data generated from \(Y_B\) are far apart (e.g. between 5 and 10 \%) then doubt is cast upon both \(Y_A\) and \(Y_B\). One may then be forced to pursue even more complex model, \(Y_C\), and then compare \(Y_B\) and \(Y_C\). Since \(Y_C\) is difficulty to verify, \(Y_B\) close to \(Y_C\) does not generate the same level of confidence as \(Y_A\) close to \(Y_B\). If \(Y_B\) is far from \(Y_C\), then one is advised to abandon the search for the non-linear operator based on only the knowledge of the individual components as shown in Eq. (1.10). One should then try to obtain the \(Y_P\), the actual vapor / liquid equilibrium (VLE), data directly from a reliable reference. \(Y_P\) (i.e. the data) may be difficult to employ directly in system (1.9). Fortunately, there are ways of approximating \(Y_P\) with a function that can be used directly in system (1.9). This is discussed in more detail in chapter 4.
1.3.3. Growth of Iteration Levels

The third mathematical difficulty with the distillation problem is that the difficulty of solving system (1.9) increases greatly when the number of components in the system exceeds two. A single level iteration scheme (a trial and error search for one unknown parameter) that solves the binary distillation problem is described in Chapter 3. The existence of a single tier iteration scheme that will solve the tertiary distillation problem is not known. If a double tier iteration scheme (trial and error search for an unknown parameter(s) nested inside a trial and error search of a separate unknown parameter) is necessary to solve tertiary distillation problem, the number of iteration loops can increase approximately by the square of the number of iterations required for the single tier iteration scheme. For example let $N_B$ represent the average number of iterations needed to solve the binary distillation problem. Then $N_T$, the average number of iterations to solve the tertiary distillation problem is:

$$N_T = N_B^2$$

Another problem with tertiary systems is encountered that can be attributed primarily to the non-linearity of the equilibrium relationships. For a binary system, the non-linear operator, $Y$, can be approximated in many cases with:

$$Y_1 = Y(X_i) = kX_i^n$$

$$Y_2 = 1-Y_1$$

$k$ and $n$ are constants chosen to fit the provided VLE data. For component $i$, $X_i$ and $Y_i$ represent the liquid and vapor phase mole fractions, respectively. If one has instead three components (tertiary), the $Y$ operator becomes:

$$Y_1 = Y(X_1,X_2)$$

$$Y_2 = Y(X_1,X_2)$$

15
A possible analog to equation (1.4) for the tertiary case is as follow:

\[ Y_1 = Y(X_1, X_2) = C_1(X_1X_2)^{\rho \ell} + A_1X_1^{\mu_1} + B_1X_2^{\mu_1} \quad (1.14) \]

\[ Y_2 = Y(X_1, X_2) = C_2(X_1X_2)^{\rho \ell} + A_2X_1^{\mu_2} + B_2X_2^{\mu_2} \]

\[ Y_3 = 1 - Y_2 - Y_1 \]

Assuming one has VLE data for the tertiary system, the number of curve fitting constants increases from two (for the binary case) to twelve. A search for twelve adjustable constants can be challenging so one generally does not see models like system (1.14). Instead one usually finds the following technique for distillation systems with three or more components with the tertiary case shown here:

\[ Y_1 = Y(X_1, T) \quad (1.15) \]

\[ Y_2 = Y(X_2, T) \]

\[ Y_3 = 1 - Y_1 - Y_2 \]

\( T \) is the temperature of the system and a function of \( X_1 \) and \( X_2 \). \( T \), unfortunately in most cases, cannot be calculated explicitly, and an iterative search must be done to find it. This is referred to as a bubble point calculation and would be expected to be done for each tray in the column. This has the net effect of adding another tier of iterations to the system (1.9), along with the increased iterations \( N_T \) noted above. In summary, the additional iteration burden of the tertiary system versus the binary system can be represented by the following equation:

\[ N_T = K*N_B^2 \]

\( K \) = the number of trays in the column

\( N_B \) = the average number of iterations expected

Further discussion of these difficulties as well as some possible simplifications that may alleviate these problems, are shown in Chapter 4. Whether one chooses to use Eqs. (1.14) or
(1.15) to determine VLE for the tertiary case, a significant calculation burden is added to the system (1.9) for this case. This is the main reason why the majority of this paper is focused on binary distillation.
CHAPTER 2

LITERATURE REVIEW OF DISTILLATION ALGORITHMS

2.1 Introduction

In this chapter, the standard algorithms for solving distillation problems will be analyzed with an emphasis on those that are most suitable with RACR. Prior to 1975, these were essentially only graphical methods. Explicit computing (non-graphical) algorithms, however, date back to the 1930s. Most notable are the legacy (pre-computers) Thiele-Geddes (TG) and Lewis-Matheson (LM) methods (Thiele and Geddes 1933; Lewis and Matheson 1932). Because of the complexity and extensive mathematical computations needed to solve problems using TG or LM, they will be considered outside pre-1975 RACR. This leaves only the graphical methods for that period. The McCabe-Thiele (MT) and Ponchon-Savarit (ST) methods were the most popular (McCabe and Thiele 1925; McCabe and Smith 1956, p. 708). As computing power for the average engineering student increased rapidly after 1975, it became possible to quickly solve equations that required multiple and/or trial and error calculations. This, ironically, has not given us a clear replacement for the graphical methods in standard undergraduate courses.
2.2 Graphical Models

2.2.1 McCabe – Thiele (MT)

2.2.1.1 McCabe – Thiele Introduction

The MT method is a non-exact (or partial) solution to a binary distillation problem. It is nearly always presented as a design problem. Since its introduction in 1925 it has become the default first-choice method for solving binary distillation problems. It also dominates as the most popular method for introducing the concepts of multi-stage distillation to engineering students.

Its effectiveness is in its graphical nature that clearly portrays critical design concepts. One of these is the impact of reflux fraction, \( R_F \), on the number of stages required to achieve a certain overhead product concentration. Liquid and vapor mole fractions can easily be located on the graph. The interplay between the operating (material balance) lines and equilibrium curve is well depicted. This graphical nature also significantly reduces the calculation burden. In short, one can understand distillation by doing the MT method whereas the opposite is true (one must understand distillation first) for nearly all other methods.

Even though the MT method is based on pre-1975 RACR methods, its dominance in engineering textbooks, which dates back to the 1930s, is undiminished to this day. The reasons for this are not very obvious. It is possible that the improvements in RACR are not enough to warrant a displacement of the MT as the default distillation method. An argument will be made below that this was probably true to about the year 2000. After 2000, however, the spreadsheet has essentially replaced paper graphs. The author believes that distillation problem solutions should now be based on algorithms meant for spreadsheets (or SC – spreadsheet code) which is within the current definition of RACR.
2.2.1.1 McCabe – Thiele Method

The usual presentation of a distillation problem meant to be solved with MT is given here. This is usually done as a design problem with these parameters:

**Input Parameters:**

- Reflux Fraction \( R_F \)
- Overhead (Top) Distillate mole fraction \( X_D \)
- Feed Quality \( Q_F \)
- Bottoms mole fraction \( X_B \)

**Output Parameters:**

- Stripping Section Vapor Rate \( V_S \)
- Minimum Number of Trays/Stages \( N_{MIN} \)
- Distillate Flow \( D \)
- Bottoms Flow \( F \)
- Feed Tray \( J_F \)

The distillate and bottoms flows \( (D \text{ and } B) \) are calculated as ratios to the feed flow, \( F \) (see Fig. 1.1). To make this obvious, we will assign \( F = 1 \). Note that \( D \text{ and } B \) must always be less than 1.

The vapor and liquid rates will also be calculated as ratios to \( F \). Feed Quality \( Q \), is:

\[
Q = \text{Feed Moles Liquid} / \text{Total Feed Moles}
\]

(2.1)

We represent the additional liquid flow applied to the feed tray as \( F_L = F(Q) = Q \).

The additional vapor applied to the tray above the feed tray will be \( F_V = F(1 - Q) = 1 - Q \).

Additional assumptions for an MT problem are that liquid enthalpy and vapor enthalpy are not functions of composition. This, coupled with the material balance constraint, creates a convenient simplification in that the vapor and liquid rates in each section of the column are constant. This is called constant molal overflow. Another effect is that there is a constant difference in vapor / liquid enthalpy that is independent of concentration. In fact, all liquid enthalpies can be assumed to be zero, and all vapor enthalpies can be assumed to be a constant without loss of generality.
Another assumption is that the equilibrium function can be approximated by plotting a set of VLE data pairs on a graph. The VLE data pairs can come from actual data or be generated by a model (e.g. Margules). The missing points are indicated by connecting the available points. Limited VLE data may require the use of a French curve.

Based on the above assumptions, several parameters can be explicitly calculated. The overall material balance is:

\[ F = B + D \quad (2.2) \]

since \( F = I \):

\[ I = B + D \quad (2.2B) \]

The overall component balance is:

\[ F(X_F) = D(X_D) + B(X_B) \quad (2.3) \]

which, based on \( F=I \) and Eq. (2.2B), gives:

\[ X_F = (1-B)X_D + (B)X_B \quad (2.3B) \]

The above equations give explicit values for the distillate and bottoms flow rates as fractions of the feed flow expressed in terms of the stream concentrations:

\[ B = (X_F - X_D)/(X_B - X_D) \quad (2.3C) \]
\[ D = (X_B - X_F)/(X_B - X_D) \quad (2.3D) \]

The rectification liquid rate \( (L_R) \) is:

\[ L_R = D(R_F/(1 - R_F)) = D(R_R) \quad (2.4) \]

where \( R_R = \) Reflux Ratio

The rectification vapor rate \( (V_R) \) can be obtained by a material balance around the condenser:

\[ V_R = D(1 + R_R) \quad (2.5) \]

A component material balance around the top of the column that cuts between any two trays in the rectification section gives the following (refer to bubble \( I \) in Fig. 1.1):
\[ V_R(Y_K) = L_R(X_{K+1}) + D(X_D) \quad (2.6) \]
\[ Y_K = (X_{K+1})(R_R/(1+R_R)) + (X_D)/(1+R_R) \quad (2.6A) \]

where \( K \) indicates a tray number in the rectification section and \( K+1 \) indicates the tray number just above.

There is a similar material balance equation that goes around the reboiler and cuts between any two trays in the stripping section (refer to bubble 3 in Fig. 1.1):

\[ L_S(X_{J+1}) = V_S(Y_J) + B(X_B) \quad (2.7) \]

\( J \) represents a tray number in the stripping section. Because of constant molal overflow, the liquid rate in the stripping section is the rectification liquid rate plus any additional liquid feed. Also, because the rectification vapor rate includes any vapor feed, the stripping vapor rate is the rectification vapor rate minus the vapor feed. This eliminates \( L_S \) and \( V_S \):

\[ (L_R + Q)(X_{J+1}) = (V_R + Q - I)(Y_J) + B(X_B) \quad (2.8) \]

Equations (2.6) and (2.8) represent the operating lines for the rectification and stripping sections respectively. All passing stream concentrations, between trays in the column, are on their applicable operating line – stripping or rectification. Since these two sections are separated by the feed tray, in actuality they never meet. The last applicable point for the stripping operating line occurs just below the feed tray at \( X_{J+1} = X_{JF} \). The last applicable point for the rectification operating line occurs just above the feed tray at \( X_{K+1} = X_{JF+1} \). In the limit, however, an infinitesimal separation can occur between the feed tray and the tray above in which essentially no concentration change occurs between the two trays. In other words, a theoretical intersection point between the two operating lines exists for this case:

\[ X_{JF} = X_{JF+1} = X_I \quad (2.9) \]
Because the vapor concentration is a function of the liquid concentration, we also have:

\[ Y_{JF} = Y_{JF+1} = Y_f \]  

(2.10)

Inserting the point \((X_f, Y_f)\) into equations (2.6) and (2.8), subtracting one equation from the other, and utilizing equation (2.3) yields:

\[ Y_f = \frac{Q/(Q-1)}{X_f/(1-Q)} \]  

(2.11)

The above implies that the intersection point also occurs along the line:

\[ Y = \frac{Q/(Q-1)}{X_f/(1-Q)} \]  

(2.12)

The above equation is known as the feed line. Equations (2.12) and (2.6A) can be solved simultaneously to identify the intersection point. This gives a value for \(X_f\) in terms of known quantities:

\[ X_f = \frac{X_d/(Q-1) + X_f/(1+R_r)/(Q(1+R_r) - R_r(Q-1))} \]  

(2.13)

\(Y_f\) can then be recovered from Eq. (2.12).

The equations above provide values for the liquid and vapor rates in both sections of the column as well as bottoms and distillate flow rates. They also provide a means for calculating the concentration of a stream provided that the corresponding passing stream concentration is known. Determination of the minimum number of trays completes the solution. The equilibrium condition is required to do this:

\[ Y = Y(X) \]  

(2.14)

The solution proceeds in domino fashion by first using the equilibrium relationship to calculate the reboiler vapor concentration \(Y_0 = Y(X_0) = Y(X_B)\). \(X_f\) is then obtained from the stripping operating equation (2.8). \(Y_f\) is then retrieved from \(Y(X_f)\). This process is repeated as many times as necessary until a value of \(Y_J\) is reached that exceeds \(Y_f\). The value of \(J\) where this occurs is the feed tray. At this point the rectification operating equation (2.6) is used to
determine the passing liquid stream concentration. This continues until $Y_j$ exceeds $X_D$. The value of $J$ at this point is the minimum number of trays, $N_{\text{MIN}}$, needed to achieve the specified separation.

It would be only coincidental if $Y_j$ were exactly $X_D$. For this reason, MT is not an exact solution to a distillation problem because it does not give an actual operating solution. One would need to adjust a parameter, for example the reflux fraction, and repeat the MT method until an exact match occurred. This does not detract, however, from its value as an engineering design tool, since having an exact operating solution is not necessary to deduce the required number of trays for a given separation.

The traditional solution to a MT problem, however, is not solved analytically (as done above), but is done graphically. Recall that the MT method was developed several decades before the sudden RACR change in the mid 1970s. The intersection point $(X_i, Y_i)$ would be revealed graphically by constructing the rectification and feed lines. The stripping line would then be drawn from this intersection point to the point where the stripping line intersects the $Y = X$ line which occurs at $X = X_B$. After drawing in the equilibrium curve, the same solution described analytically above can then be achieved graphically in a stair-stepping fashion. Figure 2.1 shows an example of a completed MT diagram.
2.2.2 Ponchon-Savarit (PS) Model

A limitation of the MT method is that it must assume that enthalpy is constant with respect to concentration. When this assumption is not valid, the graphical Ponchon-Savarit method can be used. (McCabe and Smith 1956, p. 708) The necessity of considering the energy equations in the distillation problem results in the crossing stream concentrations, \( (X_{j+1}, Y_d) \), no longer falling on a common line as in the MT method. This requires construction of a different operating line for each crossing stream (between the trays).

The PS graph is plotted on an enthalpy / concentration diagram that shows the vapor enthalpy and liquid enthalpy relationships to concentration. The equilibrium relationship between the vapor and liquid concentrations is handled, in a somewhat awkward fashion, by the use of tie lines. This requires a certain degree of subjectivity in that one must infer the slope of the tie line based on the slope of the two immediate adjacent tie lines. The difficulty is similar to
interpolating a log scale that has only a few points.

The solution to a distillation problem using PS proceeds in a similar stair-stepping fashion as MT by moving alternately from an operating line to an equilibrium tie line until an appropriate number of stages have been counted. An example of a PS diagram is shown in Figure 2.2.

PS is also a non-exact solution in that it does not give a true solution to a distillation problem as outlined in chapter 1. Although it can account for enthalpy variations, this accommodation is paid for by an increased difficulty in construction of the graph as compared to MT. A PS diagram also suffers visually when compared to an equivalent MT diagram. In other words, an MT diagram clearly shows the relationships between the equilibrium curves, operating lines and number of stages. Since the equilibrium curve is somewhat hidden in the PS diagram, its relationship to the other parameters is less apparent.
2.3 Computer Models

2.3.1 Rigorous Methods

A rigorous method is one that attempts to find the unknown parameters for a distillation problem that, when coupled with the known parameters, solve the material / energy balance and equilibrium equations (1.9). The emergence of computers after about 1950 minimized the time and effort for finding solutions.

All rigorous computer methods (RCMs), as far as is known, with the possible exception
of the algorithm presented in Chapter 3, employ traditional coding (TC) techniques. Specifically, the algorithms guess certain unknown parameters (e.g. the tray temperatures), and the remaining unknown parameters are calculated. The calculated unknown parameters are checked for errors, and this information is used to determine, presumably, a better guess for the unknown parameters. The procedure is repeated until the error is reduced to an acceptable level. TC techniques are employed because these methods almost always have nested iteration loops.

The most noted RCMs are the computerized versions of the legacy TG and LM methods. Newer methods include the Bubble Point (BP) method, the Sum Rates (SR) method and the Inside-out method (Friday and Smith 1964; Perry and Green 1997, p. 13-43; Boston and Sullivan 1974). All these methods employ complex mathematical techniques that do not simplify the core problem of the non-linear equilibrium operator. A possible exception is the Inside-out method which employs a simplified equilibrium model for part of its solution algorithm.

Since mathematics and TC methods dominate over the distillation principles, RCMs are therefore considered outside of RACR as defined in this paper.

2.3.2 Computerization of McCabe-Thiele

Because of the issues noted above for RCMs, one can, instead, find many computerized versions of the MT method. For example, Fig. 2.3 shows a screenshot of a MT plot generated by a VBA program within Microsoft Excel. This is an example is a non-proprietary WC implementation from the viewpoint of the user. It is nearly a straight implementation of MT with an added feature of allowing the user to enter a tray efficiency. This is not a RACR implementation because the algorithm uses TC methods and would be difficult to modify if one is not familiar with VBA. It was developed by J.R. Cunningham and M.B. McGann at the
University of Tennessee at Chattanooga.

Jevric also developed a spreadsheet version of the MT method (Jevric and Fayed 2002). Unlike the Cunningham model, it appears to be a pure spreadsheet version without resorting to a background TC engine. It generates a polynomial function to approximate the VLE curve. It is definitely suitable for RACR and is recommended if one is interested in obtaining all the MT parameters without resorting to graph paper.

The Wolfram model (see Fig. 2.4) is an interactive model of the MT method (Binous). The user changes input parameters by adjusting slider controls that are assigned to those parameters (e.g. feed concentration, distillation concentration and feed quality). The MT graph is nearly instantaneously redrawn with a small change in a slider. This allows one to quickly note the effects that certain parameters have on the distillation system. Unfortunately, the proprietary nature of the model limits the further analysis of this system.
Figure 2.3 Cunningham-McGann McCabe-Thiele Spreadsheet Screenshot

Figure 2.4 Wolfram MT Interactive Model (Binous)
2.4 Summary

The tremendous increase of computational power has not produced, as of yet, any notable RACR algorithms that represent clear progress from the ninety year old MT method. In fact, much attention has been focused on computerizing MT. The reasons for this appear to be that the advancement in computer technology has not solved the underlying difficulty in distillation problems. It appears that the main difficulty, as noted earlier, is the non-linear equilibrium relationships which require nested iterations to solve.
CHAPTER 3

BINARY DISTILLATION ALGORITHM FOR SPREADSHEETS

3.1 Introduction

In the previous chapter it was noted that little progress has been seen in exploiting the capabilities of RACR in solving the distillation problem with the possible exception of proprietary software like Aspen, Wolfram and ChemSep (Binous; AspenTech 2015; ChemSep 2015). These enterprises have little incentive to make their algorithms public. In any case, it is likely that their algorithms use TC methods. One can, at least, imagine the possibilities by observing the interactive display of the Wolfram MT model, and the simplicity of the MT implementation in the Jevric method (Jevric and Fayed 2002).

The following is an SC simulation algorithm that provides, unlike the MT model, an exact solution to a binary distillation problem. It also has an advantage over MT in that it can allow for changes in enthalpy with concentration (albeit linearly). It is a fast algorithm which allows it to easily handle “slider” controls on its input parameters similar to the Wolfram MT model. Because this algorithm employs only SC methods, it can be implemented with RACR.

3.2 Algorithm Details

All the assumptions for the distillation problem as outlined in Chapter 1 apply with the additional assumption that the feed enters only as a saturated liquid. The specific enthalpy operator for vapor, $H_v$, is represented as a linear function of the low boiling component mole

32
fraction:

\[ H_v(Y_j) = sY + w \]  \hspace{2cm} (3.1)

\[ Y_j = \text{vapor mole fraction} \]

\[ s, w \text{ are constants} \]

Note: Since this is a binary distillation problem, the subscript reference for the component is dropped. All mole fractions references, \( X \) and \( Y \), refer to the low boiling component only.

The specific enthalpy operator(s) for liquid, \( H_L \), is represented as a linear function of the low boiling component mole fraction:

\[ H_L(X) = aX + c \]  \hspace{2cm} (3.2)

\[ X = \text{liquid mole fraction} \]

\[ a, c \text{ are constants} \]

Note that if \( a = c = s = 0 \), then constant molal overflow applies.

The equilibrium operator, \( \gamma \), can be represented as follows:

\[ Y = Y(X) = kX^n \]  \hspace{2cm} (3.3)

\[ X = \text{liquid mole fraction} \]

\[ Y = \text{vapor mole fraction} \]

\[ k, n \text{ are constants} \]

If \( k \neq 1 \) an azeotrope exists at:

\[ X = Y = k^{(1/(1-n))} \]  \hspace{2cm} (3.4)

The liquid temperature can be expressed in terms of the liquid mole fraction, \( X \), as follows:

\[ T = \frac{u}{X^m + g} \]  \hspace{2cm} (3.5)

\[ u, m \text{ and } g \text{ are constants} \]

The above equation (3.5) is not required to solve the system of equations. It is used as a quick tool to indicate the tray temperatures without having to resort to an iterative \textit{bubble point calculation} at each tray.

The following conventions will be used:
1. \( X_J, Y_J \) refer to mole fractions of the low boiler in the liquid and vapor phases respectively with the subscript, \( J \), indicating the applicable tray number for the entire column. Note that from Eq. (3.3) that \( Y_J = Y(X_J) = kX_J^n \).

2. \( N \) refers to the number of the top tray, and also represents the total number of trays.

3. The feed tray is referenced with the index \( J_F \).

4. \( X_F, X_B, X_D \) refer to the low boiler mole fractions in the feed, bottoms and distillate, respectively.

5. \( X_1, X_2, X_3, \ldots \) etc. refer to the liquid mole fractions on each tray where \( X_I \) represents the first tray above the reboiler.

6. \( Y_1, Y_2, Y_3, \ldots \) etc. refer to the vapor mole fractions leaving each tray where \( Y_I \) represents the vapor leaving the first tray above the reboiler.

7. \( L_1, L_2, L_3, \ldots \) etc. refer to the liquid molar flows leaving each tray where \( L_I \) represents the liquid flow leaving tray \( I \). Note that bottoms flow rate, \( B = L_0 \), and that either representation may be used.

8. \( V_B = V_0 \) the molar vapor rate leaving the reboiler. \( V_1, V_2, V_3, \ldots \) etc. refer to the molar vapor rates leaving each tray.

9. \( T_B = T_0 \) is the temperature of the reboiler. \( T_1, T_2, T_3, \ldots \) etc. are the temperatures of each tray where \( T_I \) is the liquid temperature of tray \( I \), etc.

10. \( Q_B = \) the heat input rate to the reboiler.

11. \( Q_C = \) the heat removal rate in the overhead condenser.

12. \( R_F = \) the fraction of overhead vapor, \( V_N \), that is refluxed back to the column.

For this simulation distillation problem, the known (or input) parameters are either static (configuration) or dynamic.

Static (or Configuration) Inputs:

\[
N_R = \text{the number of rectification trays} \\
N_{J_F} = \text{the feed tray number} \\
\text{Note: } N = \text{total number of trays} = N_R + N_{J_F}
\]

The enthalpy constants, \( \alpha, \beta, \gamma \) and \( \omega \) (Eqs. 3.1 and 3.2).
The equilibrium equation constants, \( k \) and \( n \). (Eq. 3.3).
The temperature equation constants, \( u, g \) and \( m \). (Eq. 3.5).
A method is provided for estimating the equilibrium and temperature equation constants from known VLE data, Margules interaction parameters, Antoine's coefficients and/or infinite dilution activity coefficients. This is discussed in more detail in Chapter 4.

Dynamic (or Operator) Inputs:

\[ F = \text{molar feed rate} \]
\[ X_F = \text{mole fraction of low boiler in feed} \]
\[ Q_B = \text{heat input rate to the reboiler} \]
\[ R_F = \text{fraction refluxed} \]

Unknown (or Output) Parameters:

\[ B = \text{bottoms flow rate} \]
\[ D = \text{distillate (overhead) flow rate} \]
\[ Y_N = \text{distillate mole fraction} \]
\[ X_0 = X_B = \text{bottoms mole fraction} \]

The steps for solving the distillation problems are as follows:

**Step 1** - Guess the bottom mole fraction. Refer to this as \( X_{BG} \).

Equations representing the overall material and energy balance for the column are as follows:

\[ F X_F = B X_0 + D Y_N \quad \text{(overall component material balance)} \]  \hspace{1cm} (3.6)

\[ F = B + D \quad \text{(overall material balance)} \]  \hspace{1cm} (3.7)

\[ F(X_F a + c) + Q_B = D(Y_N a + c) + B(X_0 a + c) + Q_C \quad \text{(overall energy balance)} \]  \hspace{1cm} (3.8)

\( Q_C \) can be eliminated by doing an energy balance around the condenser:

\[ Q_C = D(-Y_N a + Y_N s - c + w)/(1-R_F) \]  \hspace{1cm} (3.9)

This results in the energy balance equation becoming:

\[ F(X_F a + c) + Q_B = D(Y_N a + c) + B(X_0 a + c) + D(-Y_N a + Y_N s - c + w)/(1-R_F) \]  \hspace{1cm} (3.10)

With \( X_0 \) set to the guessed value, \( X_{BG} \), Eqs. (3.6), (3.7) and (3.10) represent three separate equations for the unknowns, \( B, D, \) and \( Y_N \). These equations can be reduced to explicit equations for the unknowns as follows:
\[ B = \frac{(FX_{Fa} - FX_{FS} + FC - FW - Q_b R_F + Q_B)}{(X_{BGA} - X_{BGS} + c - w)} \]  \hspace{1cm} (3.11)

\[ D = \frac{(FX_{BGA} - FX_{BGS} - FX_{Fa} + FX_{FS} + Q_B R_F - Q_B)}{(X_{BGA} - X_{BGS} + c - w)} \]  \hspace{1cm} (3.12)

\[ Y_N = \beta / \delta \]  \hspace{1cm} (3.13)

where \( \beta = FX_{BGW} + FX_{FC} - FX_{FW} + Q_B X_{BG} R_F - Q_B X_{BG} - FX_{BGC} \)

\( \delta = FX_{BGA} - FX_{BGS} - FX_{Fa} + FX_{FS} + Q_B R_F - Q_B \)

However, the last two elaborate equations are not necessary once B is determined. Note that from equations (3.6) and (3.7) that:

\[ D = F - B \]  \hspace{1cm} (3.14)

\[ Y_N = \frac{(FX_F - BX_{BG})}{D} \]  \hspace{1cm} (3.15)

Once \( Y_N \) is determined it is designated as \( Y_{NT} \) to indicate that is only a trial version for the top mole fraction because it was based on the guessed value, \( X_{BG} \).

**Step 2** - Solve the tray-to-tray material and energy balances starting from the reboiler and working up to the top of the column to determine an alternate value of \( Y_N \), which will be referred to as \( Y_{NA} \) (See Fig. 1.1, Bubbles 2 and 3).

The tray material and energy balance for the column around tray \( J \) and the reboiler are as follows:

\[ L_{J+1} + F = V_J + B \]  \hspace{1cm} (material balance)  \hspace{1cm} (3.16)

\[ FX_F + L_{J+1} X_{J+1} = BX_{BG} + V_J Y_J \]  \hspace{1cm} (component material balance)  \hspace{1cm} (3.17)

\[ Q_B + L_{J+1} (X_{J+1} a + c) + F (X_{Fa} + c) = B (X_{BGA} + c) + V_J (Y_{JS} + w) \]  \hspace{1cm} (energy balance)  \hspace{1cm} (3.18)

Note the above are for \( J \geq JF \) in which the material balance includes the feed stream (Fig. 1.1, Bubble 2). If \( J < JF \) in which the material balance does not include the feed stream, then the above equations must have \( F=0 \) to be valid (Fig. 1.1, Bubble 3).
The unknowns are $X_{j+1}$, $L_J$ and $V_J$. It might appear that $Y_J$ is an unknown also, but it can calculated directly by the equilibrium condition specified in equation (1.12) as follows:

$$Y_J = Y(X_J) = kX_J^a$$  \hspace{1cm} (1.12)

$X_J$ is not unknown since it was calculated by the previous tray material and energy balance. This cascading process was started by the initial guess, $X_{BG}$.

The explicit equations for the unknowns derived from equations, (3.16), (3.17), and (3.18) are:

$$L_{J+1} = (BY_{ja} - BY_{js} - FY_{ja} + FY_{js} + Be - Bw - Fc + Fw - Q_B)/(Y_{ja} - Y_{js} + c - w)$$  \hspace{1cm} (3.20)

$$V_J = -Q_B/(Y_{ja} - Y_{js} + c - w)$$  \hspace{1cm} (3.21)

$$X_{j+1} = \omega / \varepsilon$$  \hspace{1cm} (3.22)

where

$$\omega = (BX_0Y_{ja} - BX_0Y_{js} - FX_FY_{ja} + FX_FY_{js} + BX_0c - BX_0w - FX_FC - FX_FW - Q_BY_J)$$

$$\varepsilon = (BY_{ja} - BY_{js} - FY_{ja} + FY_{js} + Be - Bw - Fc + Fw - Q_B)$$

Use of cumbersome equations (3.20) and (3.22) can be avoided by first calculating $V_J$ from equation (3.21). Then $L_{J+1}$ and $X_{j+1}$ can be solved by rearranging equations (3.16) and (3.17) as follows:

$$L_{J+1} = V_J + B - F$$  \hspace{1cm} (3.23)

$$X_{j+1} = (BX_{BG} + V_JY_J - FX_F)/L_{J+1}$$  \hspace{1cm} (3.24)

Remember that the above are for $J \geq JF$ in which the material balance includes the feed stream.

If $J < JF$, in which the material balance does not include the feed stream, then the above equations must have $F=0$ to be valid (see Fig. 1.1, Bubbles 2 and 3).

**Step 3** - Compare the trial version of $Y_{NT}$ versus the alternate version $Y_{NA}$.

Let $Y_{NE}$ designate the error between $Y_{NT}$ and $Y_{NA}$:

$$Y_{NE} = Y_{NT} - Y_{NA}$$  \hspace{1cm} (3.25)
If \( Y_{NE} > 0 \) set the current \( X_{BG} \) as the lower bound per the interval halving iteration scheme. If \( Y_{NE} < 0 \) set the current \( X_{BG} \) as the upper bound.

**Step 4** - Compute a new \( X_{BG} \) as the average of the lower and upper bounds of \( X_{BG} \) obtained in Step 3

**Step 5** - Repeat steps 1 through 4 until \( Y_{NE} \) reaches an acceptable small value.

It should be obvious that the lower and upper search bounds for \( X_{BG} \) are zero and one respectively. Based on the dynamic settings, however, the bounds can sometimes be made tighter to improve the search efficiency. This is apparent after rearranging equations (3.6), (3.7) and (3.10) to give explicit values for \( B, D \) and \( X_0 \) in terms of the dynamic settings and the overhead mole fraction, \( Y_N \).

\[
D = Q_B(1 + R_F)/(Y_{Na} - Y_{NS} + c - w) \tag{3.26}
\]

\[
B = F - D \tag{3.27}
\]

\[
X_0 = (FX_F - DY_N)/B \tag{3.28}
\]

\( Y_N \) also has lower and upper bounds of 0 and 1. By inserting each of these values into the above three equations, one obtains equations for the minimum and maximum possible values for \( X_0 \) as follows:

\[
X_{0\ maximum} = FX_F/(F - Q_B(R_F-1))/(c-w)) \tag{3.29}
\]

\[
X_{0\ minimum} = (FX_F - \omega)/(F - \omega) \tag{3.30}
\]

where \( \omega = Q_B(R_F-1))/(a-s+c-w) \)

Sometimes equations (3.29) and (3.30) offer no improvement on closing the bounds for \( X_{BG} \) in that \( X_{0\ maximum} \) may exceed 1 and/or \( X_{0\ minimum} \) may be less than zero. In that case, the algorithm should fall back to the original minimum and/or maximum bounds, 0 and 1, as appropriate. Still further improvement can be made if an azeotrope is known to exist, by using
the azeotrope value in equations (3.26), (3.27) and (3.28). For example, for the ethanol/water distillation system an azeotrope exists at:

\[ \text{Azeotrope [Ethanol/Water]} = X = Y = 0.894 \]  \hspace{1cm} (3.31)

This value, instead of \( I \), should be used to calculate the minimum value of \( X_{BG} \) (assuming the distillation system is operating below the azeotrope).

Figures 3.1 and 3.2 show an implementation of the above algorithm on the open source spreadsheet program LibreOffice Calc (Version 4). Figure 3.1 shows the top half of the spreadsheet, and Figure 3.2 shows the bottom left of the spreadsheet. The input parameters are in blue type. The first five columns, toward the middle of the sheet, represent the first column iteration. Cell C32 displays the first trial value of \( Y_{NT} \). Cell D32 displays the alternate value, \( Y_{NA} \). The difference between these values, the error, \( Y_{NE} \) is shown in Cell E32. The interval halving correction is made, and the new \( X_{BG} \) value is calculated and displayed in cell G35. Spreadsheet columns, F through J, represent the second iteration. Subsequent iterations occur every five spreadsheet columns to the right. For this implementation, nine full iterations are done (not all are shown). The final error, \( Y_{NE} \), in this case is \(-0.0004\) which means that the accuracy in the top distillation concentration is good to four significant digits.

Figure 3.3 is an implementation of the algorithm (with constant molal overflow) on Microsoft Excel with slider controls on the feed flow, feed concentration, steam input, and reflux fraction. The graph shown is a temperature profile curve of the distillation column. The temperatures are calculated using equation (3.5).
**Figure 3.1** Top Half of Algorithm Implementation in LibreOffice Calc
Figure 3.2 Bottom Half of Algorithm Implementation in LibreOffice Calc
3.3 Summary

It was shown that a robust algorithm can be implemented in a spreadsheet environment (SC) that models an exact solution to a binary distillation problem. This implementation can be equipped with interactive controls (e.g. sliders) that allow the user to quickly realize the effects of altering input parameters. It is believed that this model has applicability in education and industry and represents a step forward in showing how RACR can be used to display robust distillation problem solutions.
CHAPTER 4
EQUILIBRIUM MODELS

4.1 Introduction

Much of the burden of solving a distillation problem can be reduced by choosing an optimal equilibrium equation. Effective algorithms using RACR require an algorithm that efficiently maps liquid concentrations to their corresponding equilibrium vapor concentrations using minimal computational resources. This is the key to developing fast solutions that allow for incorporating an interactive interface as shown in the algorithm of the previous chapter.

Since the equilibrium concentrations in the liquid and vapor phases can be thought of as vector quantities, this is, in essence, a search for an equilibrium operator (EO) that is accurate and easy to mathematically deploy. As noted in chapter 1, we will designate the perfect EO as

$$Y_P: \quad (Y_1, Y_2, Y_3 \ldots Y_{N-1}) = Y_P(X_1, X_2, X_3, \ldots X_{N-1})$$  \hspace{1cm} (4.1)

Note: The subscripts refer to particular components (not tray number).

Tremendous difficulty arises, as noted in chapter 1, when there is more than one independent variable, so most of the focus in this chapter will be on equilibrium models for binary systems that have the form:

$$Y_1 = Y_P(X_1)$$  \hspace{1cm} (4.2)
4.2 Interpolation Methods

Knowledge of $Y_p$ can be gained, in an empirical sense, if one has laboratory determined equilibrium data for the particular binary system being studied at the given operating pressure of the distillation column. Perry’s Chemical Engineering Handbook (Perry’s) is one source of binary system vapor liquid equilibrium (VLE) data (Perry and Green 1997). Table 4.1 shows the ethanol / water data from this source. This table cannot provide, as expected, values for all points within the range of the VLE data. A method for estimating values between the provided data points is required. A linear interpolation algorithm could be used as follows:

Step 1: Find the Lowest Value, $J$, in Table 4.1 where $X > X_J$

Step 2: Solve for $Y(X) = (X-X_J)*(Y_{J+1}-Y_J)/(X_{J+1}-X_J) + Y_J$ \hfill (4.3)

Note: The subscript $J$ refers to a particular data pair (not components, nor trays) (see Table 4.1).

Eq. (4.3) utilizes the data pairs $(X_J, Y_J)$ and $(X_{J+1}, Y_{J+1})$ to construct a linear function in which $Y$ can be determined from $X$. Improved accuracy can be obtained by doing quadratic interpolation as follows:

Step 1: Find the Lowest Value, $J$, in Table 4.1 where $X > X_J$

Step 2: If $J<N-1$, where $N$ is the total number of data pairs, then:

$Y(X) = Y_J * L_0(X) + Y_{J+1} * L_1(X) + Y_{J+2} * L_2(X)$ \hfill (4.4)

where

$L_0(X) = (X - X_{J+1})*(X - X_{J+2})/(X_J - X_{J+1})/(X_J - X_{J+2})$
$L_1(X) = (X - X_J)*(X - X_{J+2})/(X_{J+1} - X_J)/(X_J - X_{J+2})$
$L_2(X) = (X - X_J)*(X - X_{J+1})/(X_{J+2} - X_J)/(X_{J+2} - X_{J+1})$

If $J>N-1$, where $N$ is the total number of data pairs, then let $I=J-1$:

$Y(X) = Y_I * L_0(X) + Y_{I+1} * L_1(X) + Y_{I+2} * L_2(X)$ \hfill (4.5)

where

$L_0(X) = (X - X_{I+1})*(X - X_{I+2})/(X_I - X_{I+1})/(X_I - X_{I+2})$
$L_1(X) = (X - X_I)*(X - X_{I+2})/(X_{I+1} - X_I)/(X_I - X_{I+2})$
$L_2(X) = (X - X_I)*(X - X_{I+1})/(X_{I+2} - X_I)/(X_{I+2} - X_{I+1})$

44
Cubic and higher order interpolations are not recommended because of possible errors resulting from anomalies in the curve fitting process. Linear interpolation (LI) (using Eq. 4.3) and quadratic interpolation (QI) (Using Eqs. 4.4 and 4.5) are considered generally accepted techniques for approximating an unknown function between data points. One should, however, use caution when relying upon these techniques. The approximated function may not behave in a sufficiently linear and/or quadratic manner at the point of interpolation. The suitability of using these methods can be tested for a given set of VLE data by checking the linearity and/or parabolicity at the region of interpolation. For example, suppose one is interested in obtaining \( Y \) from \( X \) using linear interpolation as follows:

\[
Y = Y(X) = (X-X_1) \frac{(Y_2-Y_1)/(X_2-X_1)}{X_2-X_1} + Y_1 \quad (4.6)
\]

where \( X_1 < X < X_2 < X_3 < X_4 \)

One can do a trial interpolation by finding the line connecting \((X_1,Y_1)\) and \((X_3,Y_3)\) and then finding a test value, \( Y_{2T} \), obtained from \( X_2 \) on this line. Then compare \( Y_{2T} \) and \( Y_2 \):

\[
Error = \text{Abs}(Y_2-Y_{2T})/Y_2 \quad (4.7)
\]

A maximum error can be set as a specification for rejecting linear interpolation. A similar approach can be used for accepting/rejecting quadratic interpolation by finding the parabola that connects \((X_1,Y_1)\), \((X_3,Y_3)\) and \((X_4,Y_4)\) and evaluating \( X_2 \) on this parabola to obtain a trial \( Y_{2T} \).

Then use Eq. (4.7) to determine the error. If the test for parabolicity is not acceptable then one should consider another method for finding the equilibrium operator.

For design distillation problems where latency is not an issue and accuracy is paramount, interpolation techniques are recommended. This is assuming, of course, that the VLE data are available and that the data pass the applicable linearity and parabolicity tests mentioned above. For simulation distillation problems, the extra computational burden of interpolation may
negatively affect the latency. For example, consider a distillation column with 30 trays, and that one is interested in seeing the effect on the overhead concentration, $Y_N$, by a change in reflux, $R_F$. Suppose that $R_F$ is moved from 0.45 to 0.55 within one second, and that ten instances of the distillation problem are solved in that one second. For every instance of the distillation problem solved, assume that ten column (tray-to-tray) iterations are required. For every iteration a call to the equilibrium function is required for each of the 30 trays. This requires $10 \times 10 \times 30 = 3000$ calls to the equilibrium function in one second. Clearly, the equilibrium calculation should be done quickly. Ideally, a single line of code (LOC) function is desired.

For simulation and engineering distillation problems, interpolation algorithms have challenges in creating the applicable code under RACR. The inherent nature of the interpolation algorithm suggests that it is best done with traditional coding techniques. It is theoretically possible to embed an interpolation algorithm within a spreadsheet distillation problem, but this would require a very complicated equation going into one cell. Possibly some other technique can be used to transfer the interpolation burden to another part of the spreadsheet. Because of the advanced coding skills required, the author believes that equilibrium function algorithms that involve interpolation should not be considered part of RACR.

### 4.3 Single Line Equilibrium Operators

The following is an analysis of equilibrium operators that are believed suitable for application to distillation problems solved with RACR. They all can be implemented as a single entry into a spreadsheet cell. They are discussed in order of the easiest to hardest to implement.
4.3.1 Relative Volatility (RV)

The simplest equilibrium function is the single parameter relative volatility equation. It comes about by making the following assumption:

\[ \alpha_J = \frac{Y_J/X_J}{Y_N/X_N} = \text{relative volatility} = \text{constant (independent of temperature)} \]  \hspace{1cm} (4.8)

\( N \) is the number of components and also represents the component with the least volatility.

\( J \) represents a particular component. For a binary system this becomes:

\[ \alpha_I = \frac{Y_I/X_I}{(1-Y_I)/(1-X_I)} \]  \hspace{1cm} (4.9)

Note: The subscript 1 may be dropped since for binary systems it always refers to the most volatile component.

Rearranging:

\[ Y_I = \alpha X_I/(X_I*(\alpha - 1) + 1) \]  \hspace{1cm} (4.10)

For an ideal system, the relativity volatility can be determined by with:

\[ \alpha_I = P^{*I}/P^{*2} \]  \hspace{1cm} (4.11)

Where \( P^{*I} \) and \( P^{*2} \) represent the vapor pressures of pure components 1 and 2 respectively.

Equation (4.11) implies a test of the constancy of the relative volatility over the desired distillation temperature range. This is illustrated by replacing the vapor pressure terms with their Antoine equation counterparts as follows:

\[ P^{*I} = 10^{A_I}/10^{(B_I/(C_I + T))} \]
\[ P^{*2} = 10^{A_2}/10^{(B_2/(C_2 + T))} \]

\[ \alpha_I = 10^{A_I}/10^{(B_I/(C_I + T))}/(10^{A_2}/10^{(B_2/(C_2 + T))}) \]  \hspace{1cm} (4.12)

where \( A_I, B_I, C_I \) and \( A_2, B_2, C_2 \) are the Antoine coefficients for components 1 and 2 respectively. \( T \) is the temperature. By inspection of equation (4.12) one can see for temperature independence to hold, that we need \( B_2 \approx B_I \) and \( C_2 \approx C_I \). Only variation is allowed in \( A \). That is, only \( A_I \neq A_2 \) is acceptable. If this test fails, one could explicitly calculate the relative
volatility at each end of the distillation temperature range. Call these two relative volatilities, $\alpha_H$, \textit{relative volatility high} and $\alpha_L$, \textit{relative volatility low}. One could use equation (4.10) if the following error is less than a predefined limit:

$$\text{Error} = \text{Abs}(\alpha_H - \alpha_L) / \alpha_H$$

(4.13)

Equation (4.12) is probably the most direct method for finding relativity volatility between two components if VLE data are lacking. The ideal assumption must also be valid. That is, equation (1.7) must be applicable. There is no direct and easy method for deciding the applicability of equation (1.7) in the absence of VLE data. The only guidance is that the components must be chemically similar.

If VLE data are available, the relative volatility should be calculated directly using equation (4.9) at each available point within the distillation temperature range. One should only consider using equation (4.10) if the variance in the relative volatility is within an acceptable limit.

\textbf{4.3.2 Exponential Azeotropic Model (EA)}

One noticeable disadvantage of the RV model, is that it cannot handle an azeotrope, in that, $Y=X$ only occurs at $X=1$ and $X=0$. The following two parameter model discussed in chapter 3:

$$Y = Y(X) = kX^n$$

(1.12)

has an azeotrope at:

$$X_{AZ} = Y_{AZ} = k^{(1/(1-n))}$$

(4.14)

if $k \neq 1$ and $n \neq 1$. 

48
To determine \( k \) and \( n \) for a given system one must have access to VLE data or estimates of VLE data from one of the more advanced models discussed below. A minimum of two data pairs, \((X_1,Y_1)\) and \((X_2,Y_2)\), where \(X_2 > X_1\), is required. The subscripts refer to particular data pairs from a set of VLE data (not trays, nor components) Additional data pairs can be used to validate the model. The following guidelines should be applied to ensure best results:

1. Do not use \((0,0)\) as a data point since this is calculated automatically by the model.

2. Do not use \((1,1)\) as a data point since this model cannot resolve it and the azeotrope simultaneously because \( k \neq 1 \). This model should not be used if the distillation range is near \( X=1 \). See the Exponential Non-Azeotropic Model below if the distillation range is near \( X=1 \).

3. If the distillation range is near a known azeotrope, the azeotrope should be used as a data pair \((X_{AZ}, Y_{AZ})\). Note that \( X_{AZ} = Y_{AZ} \).

4. If there is no known azeotrope, the model will infer a “pseudo-azeotrope” which may not be valid. If this is the case, it is recommended that the distillation range stay within \( X_1 < X < X_2 \).

To determine \( k \) and \( n \), insert the data pairs into Eq. (1.12):

\[
Y_1 = kX_1^n \\
Y_2 = kX_2^n
\]  

(4.15)  

(4.16)

Eliminating \( k \) one obtains an equation for \( n \):

\[
n = \frac{\ln(Y_1/Y_2)}{\ln(X_1/X_2)}
\]  

(4.17)

\( k \) can then be recovered by inserting \( n \) into either equation (4.15) or (4.16):

\[
k = Y_2/X_2^n
\]  

(4.18)

The validity of the model can be checked by inserting other known data pairs, \((X_3,Y_3), (X_4, Y_4), \ldots (X_N,Y_N)\). These other data pairs should be within the range \( 0 < X < X_{AZ} \). \( X_{AZ} \) is calculated from equation (4.14). To improve success of this model, only the data pairs within the distillation range should be used.
The average difference from the model can be determined by the following:

\[
\text{Average Difference} = \left( \sum_{j=3}^{N} \left( \left( \frac{Y_j - K X_j^n}{(N-2)^{1/p}} \right)^p \right) \right)^{1/p}
\]  

where \( p \geq 1 \) is an arbitrary constant.

A larger \( p \) gives greater weight to the instances of greater differences in the data set.

The model can be rejected if the average difference for specified value of \( p \) is not within acceptable limits.

### 4.3.3 Exponential Non-azeotropic Model (ENA)

This is similar to the exponential azeotropic model discussed above with the difference that \( k=1 \), which eliminates the azeotrope. It is a one parameter model similar to the relative volatility model.

\[
Y_i = X_i^n
\]  

with \( n < 1 \)

Only one data pair is needed to find \( n \):

\[
n = \frac{\ln(Y_i)}{\ln(X_i)}
\]  

The data pair, \((X_i, Y_i)\), should generally be selected from the middle of the data range.

It is an alternative to the RV model. Configured to the same data point \((X_i, Y_i)\), the ENA model calculates greater values for \( Y \) for \( X < X_i \) compared to the RV model.

The model can be validated in a similar fashion to the EA model with equation (4.19) and setting \( k = 1 \).
4.3.4 Standard Ideal Model with Temperature Estimation

An obvious question may be why not use the ideal law equation (1.7) (also known as Raoult's Law) directly for equilibrium concentration calculations. The reason is that the pure component vapor pressures are functions of temperature, $T$. Temperature is also a function of concentrations for a given distillation problem. Why not insert this function into Eq. (1.7)?

This brings up the fundamental difficulty when solving VLE problems:

Temperature can rarely (if ever) be expressed as an explicit function of mixture concentrations without making certain assumptions.

This is a characteristic of a one-way function. The easy direction is from temperature to concentrations and the opposite, concentrations to temperature, is the hard direction.

Unfortunately, good solutions to distillation problems often require frequent calculations to determine temperature. This is best illustrated by substituting Antoine's equation for the vapor pressure, $P_1^*$, into Eq. (1.7):

$$Y_1 = X_1^* \left(10^{A1/10^{B1/(C1+T)}}\right)/P$$

(4.22)

where $P = \text{system pressure} = \text{constant (per the assumption for distillation problems)}$

and $A_1, B_1,$ and $C_1$ are the Antoine coefficients for the particular component.

$T$ can only be expressed in terms of $X_1$ implicitly:

$$P = X_1^* \left(10^{A1/10^{B1/(C1+T)}}\right) + \left(1-X_1\right)^*\left(10^{A2/10^{B2/(C2+T)}}\right)$$

(4.23)

where the new expression added represents the contribution to the total pressure by the second component.

Equation (4.23) requires an iterative method to solve. Once $T$ is found, $Y_1$ can easily be determined by substituting $T$ and $X_1$ in equation (4.22). Many robust solutions to distillation problems do exactly this. This does not, however, meet our standards under RACR because of the difficulty (as mentioned above) of embedding another iteration level in a spreadsheet.

51
A way out of this difficulty is realizing that equation (4.23) can be used to generate a table of \((X,T)\) data pairs. This needs to be done only once for a particular system. From these data, we attempt to create a reasonably approximate explicit function for \(T\) in terms of \(X\). This function, \(T(X)\), can then be inserted into equation (4.22) thus eliminating \(T\) and creating a one line equilibrium function.

One model equation that works well for the ethanol/water system (table 4.1), which implies possible success for other systems, is:

\[
T = T[X] = \frac{u}{X^m + g}
\]

where \(u\), \(m\) and \(g\) are constants.

Three data pairs, \((X_1, T_1)\), \((X_2, T_2)\), \((X_3, T_3)\), are needed to determine the constants. These can be obtained from a trial and error solution to equation (4.23) or from actual VLE data. Inserting these data pairs into Eq. (3.5) and rearranging gives:

\[
\begin{align*}
    u &= (X_1^m - X_2^m)/(1/T_1 - 1/T_3) \\
    g &= u/T_3 - X_3^m \\
    \theta &= X_2^m + g - u/T_2
\end{align*}
\]

An initial guess for \(m\) is entered into Eq. (4.24) to obtain a corresponding trial version of \(u\).

Both \(u\) and \(m\) are entered into Eq. (4.25) to obtain a trial version of \(g\). All three constants are entered into Eq. (4.26) for verification. Corrections to \(m\) are made and the process repeated until the result of equation (4.26) is sufficiently close to zero.

Additional data pairs, \((X_4, T_4)\), ... \((X_N, T_N)\), can be used for model verification with an analog of equation (4.19):

\[
Average\ Difference = \left( \left( \sum_{j=4}^{N} \left( \left( T_j - T[X] \right) \right)^p \right) / \left( N - 3 \right) \right)^{1/p}
\]

(4.27)
Substituting Eq. (3.5) into Eq. (4.22) gives the desired temperature-free equation (in spreadsheet notation):

\[ Y_i = X_i \times 10 \cap \frac{(A1 - (B1^*X_i^\cap m + B1^*g)/(C1^*X_i^\cap m + C1^*g + u))/P}{P} \quad (4.29) \]

One should be aware that neither Eq. (4.23) nor Eq. (4.29) offers an explicit way to determine the location of any azeotropes. Substituting \( X_{AZ} \) for both \( X_i \) and \( Y_i \) in equation (4.29) gives an implicit equation where one can find any azeotropes by a suitable trial and error method:

\[ 0 = X_{AZ} - X_{AZ} \times 10 \cap \frac{(A1 - (B1^*X_{AZ}^\cap m + B1^*g)/(C1^*X_{AZ}^\cap m + C1^*g + u))/P}{P} \quad (4.30) \]

The data points generated from equations (4.22) and (4.23) can be used to create one of the simpler equilibrium functions discussed above. If the data are believed to be azeotrope-free, the RV or ENA model can be tried, otherwise, the EA model is suggested. These models should be verified by using the techniques mentioned.

Remember that equations derived in this section were based on the applicability of the ideal equilibrium equation (1.7). If one doubts its applicability one should consider one of the models discussed above that are based on actual VLE data. Failing this, one may need to consider the next model discussed -- Margules (Non-Ideal) Model with Temperature Estimation.

### 4.3.5 Margules Non-Ideal Model with Temperature Estimation (MNIMTE)

Recall the non-ideal equilibrium equation from Chapter 1:

\[ Y_iP = \gamma_iX_iP_i^* \quad (1.8) \]

Some binary non-ideal systems are modeled successfully with the above equation and the Margules model for the activity coefficients as follows (Perry and Green 1997, p. 13-21):

\[ \gamma_1 = \exp((A_{12} + 2(A_{21} - A_{12})X_1X_2) \quad (4.31) \]

\[ \gamma_2 = \exp((A_{21} + 2(A_{12} - A_{21})X_2X_1) \quad (4.32) \]
where interaction parameter, $A_{12}$, is the natural log of the limiting activity coefficient for component $1$ (i.e. as $X_1 \to 0$) and interaction parameter, $A_{21}$, is the natural log of the limiting activity coefficient for component $2$ (i.e. as $X_2 \to 0$)

The limiting activity coefficients will need to be obtained from a reference (e.g. Perry's) (Perry and Green 1997, p. 13-20). Alternatively, they can be estimated by knowledge of the molecular structure of the components using UNIFAC or other models (Poling, Prausnitz et al. 2001, p. 8.75).

Substituting Eqs. (4.31) and (4.32) into Eq. (1.8) for each component and eliminating $X_2$ gives:

$$Y_1 = \exp((A_{12} + 2(A_{21}-A_{12})*X_1*(1-X_1)^2) * X_1 * (10^{A1/10^{B1/(C1+T)}})/P$$  \hspace{1cm} (4.33)

$$Y_2 = \exp((A_{21} + 2(A_{12}-A_{21})*(1-X_1)*X_1^2) * (1-X_1) * (10^{A2/10^{B2/(C2+T)}})/P$$  \hspace{1cm} (4.34)

with the requirement, as in the ideal case, that:

$$I = Y_1 + Y_2$$

This results in a single implicit equation for $T$:

$$\exp((A_{12} + 2(A_{21}-A_{12})*X_1*(1-X_1)^2) * X_1 * (10^{A1/10^{B1/(C1+T)}})/P = I - \exp((A_{21} + 2(A_{12}-A_{21})*(1-X_1)*X_1^2) * (1-X_1) * (10^{A2/10^{B2/(C2+T)}})/P$$  \hspace{1cm} (4.35)

The above equation is the non-ideal analog to equation (4.23). It can then be used to generate a series of data pairs $(X_i, T_i), (X_2, T_2), \ldots (X_N, T_N)$. Using three of these data pairs, an explicit function for the temperature can be generated by using equations (4.24), (4.25), (4.26) as shown in the ideal case.

Insertion of this explicit temperature function into Eq. (4.33) gives:

$$Y_i = \exp((A_{12}+2(A_{21}-A_{12})*X_i*(1-X_i)^2) * X_i * (10^{A1-(B1*X_i)+m+B1*g)/(C1*X_i*m+C1*g+u)})/P$$ \hspace{1cm} (4.36)

Azeotropes can only be found by trial and error methods using equations (4.35) or (4.36).

The data points generated from equations, (4.34) and (4.35), can be used to create one of the simpler equilibrium functions discussed above. If the data are believed to be azeotrope-free,
then the RV or ENA model can be tried, otherwise, the EA model is suggested. These models should be verified by using the techniques mentioned.

4.3.6 Comparison of Binary Single Line Equilibrium Operators

Tables 4.2 through 4.4 show sample implementations of the above algorithms. Table 4.2 compares the EA model to actual ethanol/water data given in Table 4.1. The average difference of the error using equation (4.19) is 0.052 (about 5.2%).

Table 4.3 shows the ENA model and the RV model versus actual methanol/water data from Perry’s (Perry and Green 1997, p. 13-13). The RV model gives an average difference of about 8.5%. The ENA model gives an improved value of 4.3%.

Finally, Table 4.4 shows and implementation of the MNIMTE model on the ethanol/water system. Spreadsheet cell, T22, shows the average difference of the $Y$ values from the MNIMTE model (Eq. 4.36) versus the $Y$ values generated by an iterative search of the Margules model (Eq. 4.35) at each data point. This average difference is about 0.6% which is very close to the implicit Margules model. Cell, U22, shows that the MNIMTE model has an average difference of about 1.1% from the actual data which is a significant improvement over the EA model (5.2%) for the same data.
Table 4.1

Ethanol / Water VLE data

(Perry and Green 1997, p. 13-12)

<table>
<thead>
<tr>
<th>Index (J)</th>
<th>Temperature (C)</th>
<th>Liquid Mole Fraction (Ethanol)</th>
<th>Vapor Mole Fraction (Ethanol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>95.5</td>
<td>0.019</td>
<td>0.17</td>
</tr>
<tr>
<td>2</td>
<td>89</td>
<td>0.0721</td>
<td>0.3891</td>
</tr>
<tr>
<td>3</td>
<td>86.7</td>
<td>0.0966</td>
<td>0.4375</td>
</tr>
<tr>
<td>4</td>
<td>85.3</td>
<td>0.1238</td>
<td>0.4704</td>
</tr>
<tr>
<td>5</td>
<td>84.1</td>
<td>0.1661</td>
<td>0.5089</td>
</tr>
<tr>
<td>6</td>
<td>82.7</td>
<td>0.2337</td>
<td>0.5445</td>
</tr>
<tr>
<td>7</td>
<td>82.3</td>
<td>0.2608</td>
<td>0.558</td>
</tr>
<tr>
<td>8</td>
<td>81.5</td>
<td>0.3273</td>
<td>0.5826</td>
</tr>
<tr>
<td>9</td>
<td>80.7</td>
<td>0.3965</td>
<td>0.6122</td>
</tr>
<tr>
<td>10</td>
<td>79.8</td>
<td>0.5079</td>
<td>0.6564</td>
</tr>
<tr>
<td>11</td>
<td>79.7</td>
<td>0.5198</td>
<td>0.6599</td>
</tr>
<tr>
<td>12</td>
<td>79.3</td>
<td>0.5732</td>
<td>0.6841</td>
</tr>
<tr>
<td>13</td>
<td>78.74</td>
<td>0.6763</td>
<td>0.7385</td>
</tr>
<tr>
<td>14</td>
<td>78.41</td>
<td>0.7472</td>
<td>0.7815</td>
</tr>
<tr>
<td>15</td>
<td>78.15</td>
<td>0.8943</td>
<td>0.8943</td>
</tr>
</tbody>
</table>
Table 4.2
Comparison of Single Line Azeotropic Equilibrium Model to Actual Data

Ethanol / Water

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>J</td>
<td>T</td>
<td>X</td>
<td>Y</td>
<td>Y EA</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>85.5</td>
<td>0.016</td>
<td>0.17</td>
<td>0.215</td>
</tr>
<tr>
<td>7</td>
<td>2</td>
<td>86</td>
<td>0.0721</td>
<td>0.3891</td>
<td>0.352</td>
</tr>
<tr>
<td>8</td>
<td>3</td>
<td>86.7</td>
<td>0.0966</td>
<td>0.4375</td>
<td>0.365</td>
</tr>
<tr>
<td>9</td>
<td>4</td>
<td>85.3</td>
<td>0.1238</td>
<td>0.4704</td>
<td>0.430</td>
</tr>
<tr>
<td>10</td>
<td>5</td>
<td>84.1</td>
<td>0.1661</td>
<td>0.5069</td>
<td>0.460</td>
</tr>
<tr>
<td>11</td>
<td>6</td>
<td>82.7</td>
<td>0.2337</td>
<td>0.5445</td>
<td>0.544</td>
</tr>
<tr>
<td>12</td>
<td>7</td>
<td>82.9</td>
<td>0.2698</td>
<td>0.5518</td>
<td>0.567</td>
</tr>
<tr>
<td>13</td>
<td>8</td>
<td>81.5</td>
<td>0.3273</td>
<td>0.5626</td>
<td>0.617</td>
</tr>
<tr>
<td>14</td>
<td>9</td>
<td>80.7</td>
<td>0.3905</td>
<td>0.6122</td>
<td>0.682</td>
</tr>
<tr>
<td>15</td>
<td>10</td>
<td>79.8</td>
<td>0.5179</td>
<td>0.6564</td>
<td>0.725</td>
</tr>
<tr>
<td>16</td>
<td>11</td>
<td>79.7</td>
<td>0.5198</td>
<td>0.6599</td>
<td>0.732</td>
</tr>
<tr>
<td>17</td>
<td>12</td>
<td>79.3</td>
<td>0.5532</td>
<td>0.6841</td>
<td>0.750</td>
</tr>
<tr>
<td>18</td>
<td>13</td>
<td>78.3</td>
<td>0.6752</td>
<td>0.7385</td>
<td>0.826</td>
</tr>
<tr>
<td>19</td>
<td>14</td>
<td>78.41</td>
<td>0.7472</td>
<td>0.7815</td>
<td>0.837</td>
</tr>
<tr>
<td>20</td>
<td>15</td>
<td>78.75</td>
<td>0.8343</td>
<td>0.8943</td>
<td>0.864</td>
</tr>
</tbody>
</table>

Check Points: 13
### Table 4.3
Comparison of Single Line Non-azeotrop Model to RV Model and Actual Data

**Methanol / Water**

<p>| | | | | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>J</td>
<td>0.05</td>
<td>0.25</td>
<td>0.5</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>8</td>
<td>9</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Actual</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>D</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>B</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: The table contains data for various parameters and their comparisons between different models and actual data for methanol/water system.
### Table 4.4

**Margules Non-Ideal Equilibrium Model with Temperature Estimation**

**Ethanol / Water**

|   | G | H | I | J | K | L | M | N | O | P | Q | R | S | T | U | V | W | X | Y | Z |
| 6 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 7 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 8 | 1.1328472 | 1.0329042 | 0.9671198 | 0.8346032 | 0.7190882 | 0.6284038 | 0.5523456 | 0.4923054 | 0.4416306 | 0.3964542 | 0.3585004 | 0.3281800 | 0.3046204 | 0.2870608 | 0.2746504 | 0.2660504 | 0.2597504 | 0.2548504 | 0.2497504 | 0.2456504 | 0.2420504 |
| 9 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 10 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 11 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 12 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 13 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 14 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 15 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 16 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 17 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 18 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 19 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |
| 20 |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |   |

**Exploit Equation**

```plaintext
x1 = 0.199762, x2 = 3.82423, T1 = 95.558162, T2 = 95.588162
```

**Actual Data**

- **Squared**
  - 0.000618
  - 0.001156406

---

59
4.3.7 Tertiary Single Line Equilibrium Operator

The following is a technique for creating an explicit temperature-free equilibrium operator for a three component (tertiary) system. Because of its complexity, we will only address ideal systems.

For the tertiary system, \( N=3 \), so equation (4.1) reduces to:

\[
(Y_1, Y_2) = Y_P(X_1, X_2)
\]  
(4.37)

Applying Antoine's equation as done in the ideal binary case gives:

\[
Y_1 = X_1 \cdot (10^{A_1}/10^{B_1/(C_1+T)})/P
\]  
(4.38)

\[
Y_2 = X_2 \cdot (10^{A_2}/10^{B_2/(C_2+T)})/P
\]  
(4.39)

\[
Y_3 = X_3 \cdot (10^{A_3}/10^{B_3/(C_3+T)})/P
\]  
(4.40)

The implicit equation for temperature is:

\[
P = X_1 \cdot (10^{A_1}/10^{B_1/(C_1+T)}) + X_2 \cdot (10^{A_2}/10^{B_2/(C_2+T)}) + (1-X_1-X_2) \cdot (10^{A_3}/10^{B_3/(C_3+T)})
\]  
(4.41)

Equation (3.5) cannot be used in this case because the temperature is now also dependent on \( X_2 \).

In other words, we need an explicit function of the temperature in the form:

\[
T = T(X_1, X_2)
\]  
(4.42)

The route pursued here is to replace the problematic Antoine expressions for vapor pressure with an approximate quadratic function. This is made easier by making note of the fact that the approximation need only work over the expected distillation range. This is typically much smaller than the applicable range of the Antoine equation. The form of the equations would be:

\[
P* = a_i T^2 + b_i T + c_i
\]  
(4.43)

\[
P* = a_2 T^2 + b_2 T + c_2
\]  
(4.44)

\[
P* = a_3 T^2 + b_3 T + c_3
\]  
(4.45)

The constants \( a_i, b_i, \) and \( c_i \) (\( i = \) component number) are curve fitting constants that cause a parabola to pass through the points \((T_{LOW}, P*_{i}), (T_{MID}, P*_{i}), (T_{HIGH}, P*_{i})\). \( T_{LOW}, T_{MID} \) and \( T_{HIGH} \) represent the low, middle and high temperatures in the distillation range. These constants
can be determined by standard linear algebra techniques for solving simultaneous equations.

Substituting equations (4.43), (4.44) and (4.45) into Eq. (4.41) to replace the Antoine expressions gives:

\[ P = X_1^* (a_1 T^2 + b_1 T + c_1) + X_2^* (a_2 T^2 + b_2 T + c_2) + (1 - X_1 - X_2)^* (a_3 T^2 + b_3 T + c_3) \]  

(4.46)

Rearranging gives:

\[ 0 = (X_1^* a_1 + X_2^* a_2 + (1 - X_1 - X_2)^* a_3) T^2 + (X_1^* b_1 + X_2^* b_2 + (1 - X_1 - X_2)^* b_3) T + (X_1^* c_1 + X_2^* c_2 + (1 - X_1 - X_2)^* c_3 - P) \]  

(4.47)

Applying the quadratic equation gives us an explicit function for the temperature:

\[ T = \frac{(b^2 - 4*a*c)^{1/2} - b}{2*a} \]  

(4.48)

where

\[ a = X_1^* a_1 + X_2^* a_2 + (1 - X_1 - X_2)^* a_3 \]  

(4.49)

\[ b = X_1^* b_1 + X_2^* b_2 + (1 - X_1 - X_2)^* b_3 \]  

(4.50)

\[ c = X_1^* c_1 + X_2^* c_2 + (1 - X_1 - X_2)^* c_3 - P \]  

(4.51)

Inserting equations (4.43) and (4.44) into the ideal equilibrium equation (1.7) gives functions for \( Y_1 \) and \( Y_2 \) that are only functions of \( X_1 \) and \( X_2 \) since \( T \) is obtained from equation (4.48):

\[ Y_1 = X_1^* \frac{(a T^2 + b T + c)}{P} \]  

(4.52)

\[ Y_2 = X_2^* \frac{(a T^2 + b T + c)}{P} \]  

(4.53)

where \( a, b, c, T \) are determined from equations, (4.49), (4.50), (4.51) and (4.48) respectively.

### 4.4 Applicability and Summary

The above shows several methods for generating single line equilibrium functions that are applicable to binary systems and can be deployed with RACR. Means for checking the validity of the models was also shown. The last model shown is applicable to tertiary and higher order systems as long as the vapor pressures can be modeled with a quadratic equation within the distillation range.
CHAPTER 5
DISCUSSION AND CONCLUSIONS

5.1 Summary

Methods for solving distillation problems that can be deployed on readily available computing resources (RACR), have changed little since the introduction of the McCabe-Thiele method in 1926. The slow progression has occurred in spite of the tremendous increases in the power and availability of computing resources since the mid 1970s. Instead, most new methods are nearly identical, or slightly modified, deployments of the McCabe-Thiele method on spreadsheets (Jevric) or proprietary platforms (Wolfram).

A new spreadsheet model was presented that has significant improvements over the McCabe-Thiele method. It fully solves the binary distillation problem in that it gives the correct parameters for a given distillation column operating instance. It also can allow for enthalpy changes as a function of concentration -- although this is done as a linear approximation. The model incorporates explicit functions for the equilibrium condition that greatly increases the speed of convergence in solving a distillation problem. This allows for displaying a progression of distillation problem solutions so that one can see the influence of changing input parameters almost instantaneously.

The new model can be used in an educational setting to convey the principles of distillation to operators who may only be interested in the capabilities of existing distillation equipment. It can also be used by engineers for designing new distillation systems, who are
interested in obtaining more detailed information beyond that provided by the McCabe-Thiele system, without having to resort to proprietary computing resources.

5.2 Conclusions

The following conclusions can be made:

1. Readily available computing resources now allow for robust solutions to the binary distillation problem that represent significant improvements over traditional methods like McCabe-Thiele.

2. These solutions, unlike the McCabe-Thiele method, solve all the material balances.

3. They incorporate explicit equilibrium functions that allow these distillation solution algorithms to be easily deployed on spreadsheets.

4. The distillation solutions can be used in operations and engineering settings.

5.3 Recommendations for Further Study

Although an algorithm for generating explicit multi-component equilibrium functions was presented in Chapter four, these types of systems presented other issues that were too complex to discuss here. The main problem with higher ordered systems is the difficulty in determining improved trial parameters after a column iteration. This can be attributed to azeotropes and the residual curve. In the binary case, the location of azeotropes is usually known and can be avoided. In this way, the low boiler always remains the low boiler and more reliable guesses in trial parameters can be made based on previous iterations. In the tertiary and higher ordered cases, the knowledge gained after an iteration may offer little direct guidance on making an improved guess of the trial parameters. Full knowledge of the partitioning direction of the components, as functions of concentration(s), and throughout the distillation range, is needed to alleviate this.
It is also possible that as readily available computing resources increase in power that a Monte-Carlo type search can be done to solve multi-component distillation problems on a spreadsheet. For example, 1000 randomly generated guesses of the column state can be done at once. Another 1000 iterations can be done within the best or “hot” zone of these iterations. The level of iterations can be extended to whatever depth is needed to find a suitable solution. More work would be needed to test this possibility.
REFERENCES


VITA

Robert Bruce Coulter was born in Valley, Alabama but raised in northwest Florida. After attending Pensacola State College for two years he transferred to Auburn University and earned a bachelor degree in chemical engineering in 1979. His senior project at Auburn involved the creation of a FORTRAN coded Fenske-Underwood Multicomponent distillation model on an IBM 370 computer. He worked as a process and/or project engineer at Ampex Corporation, Graham Magnetics and Tandy Magnetics in the magnetic tape industry from 1980 to 1991. Much of his work at these companies involved wet milling of iron oxide slurries, filtration, solvent recovery (via carbon adsorption) and distillation. From 1991 to 2011, he worked in various roles in the chemical industry focusing mainly on environmental and process safety issues. For the last four years, he has been employed at Chattanooga State Community College where he is an assistant professor and the faculty lead for the chemical engineering technology program. He is a licensed professional engineer in the states of Tennessee and Florida. He earned a Master of Science: Engineering degree from the University of Tennessee at Chattanooga in 2015.