

**MODELLING AND SIMULATION OF  
MULTICOMPONENT BATCH  
DISTILLATION (NON-IDEAL VLE)  
USING A JAVA PROGRAM  
CASE OF METHYL TERTIARY BUTYL ETHER –  
METHANOL – OCTANE MIXTURE**

**By  
98/7099EH  
DANIEL, OLABISI D.**

**DEPARTMENT OF CHEMICAL ENGINEERING  
SCHOOL OF ENGINEERING AND ENGINEERING TECHNOLOGY  
FEDERAL UNIVERSITY OF TECHNOLOGY,  
MINNA, NIGER STATE**

**NOVEMBER 2004**

**MODELLING AND SIMULATION OF  
MULTICOMPONENT BATCH  
DISTILLATION (NON-IDEAL VLE)  
USING A JAVA PROGRAM  
CASE OF METHYL TERTIARY BUTYL ETHER –  
METHANOL – OCTANE MIXTURE**

**By  
98/7099EH  
DANIEL, OLABISI D.**

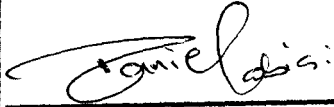
**DEPARTMENT OF CHEMICAL ENGINEERING  
SCHOOL OF ENGINEERING AND ENGINEERING TECHNOLOGY  
FEDERAL UNIVERSITY OF TECHNOLOGY,  
MINNA, NIGER STATE**

**IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF  
CHELOR OF ENGINEERING (B. ENG) DEGREE IN CHEMICAL ENGINEERING**

**NOVEMBER 2004**

# DECLARATION

here by declare that this project work is my original work and has never been submitted else where before now.



**Daniel, Olabisi D.**

23	11	04
Date		

## CERTIFICATION

is is to certify that this project titled "Modeling and Simulation of a Multicomponent Batch Distillation Column (Non-Ideal VLE) using a Java Program Case of Methyl Tertiary Butyl Ether – Methanol -- Octane Mixture" was carried by Daniel, Olabisi D. under the supervision of Engineer Elizabeth Eterigho and submitted to Chemical Engineering Department, Federal University Of Technology Minna, in partial fulfillment of the requirement for the award of Bachelor Of Engineering (B.Eng) Degree In Chemical Engineering.



**Engineer Elizabeth Eterigho**

*Project Supervisor*

22<sup>nd</sup> / 11 / 07

*Date*

---

**Dr. Agberuagba**

*Head of department*

---

*Date*

---

*External examiner*

---

*Date*

## **DEDICATION**

**This project is dedicated to my Lord and personal Savior Jesus Christ who has shown me the kind of love no one else can and has given me eternal life. To my wonderful parents Mr. & Mrs. C.F Daniel.**

## **ACKNOWLEDGEMENT**

First and foremost my sincere thanks go to the Almighty God who begun this good work and has brought me through to the end safely.

I am grateful to Engineer(Mrs) Elizabeth Eterigho for all the time and effort she put into this project. Without her knowledge, help and trust the results now obtained would not have been. I would also want to say a heartfelt thank you to Mr. Imeh for his guidance and input in my project.

I would like to thank my parents for giving me the opportunity to come to Federal University of Technology, their prayers, love and support has brought me to the end of this program.

For support and encouragement I would also like to thank all my friends who have been there for me when it really mattered the most. Ill mention just a few, Alozie, Gloria, Ibrahim, Kpam, Chehor, Jumoke, Annie, Rasaan, Kigsley, Seun, Twisty, Seye, Teni, Imoh, Nancy, Alhamdu, Rotimi. A big thank you goes to the Living Vessels and the Fellowship of Christian Students for input you have made in my life.

## NOMENCLATURE

: constant-volume holdup

: Antoine Constant

: Antoine Constant

: Antoine Constant

$y_{N+1}^0$  : initial molar charge to reboiler

: total pressure(101.3kPa) [Pa]

$p_i^{\text{sat}}$  : vapor pressure of pure component  $i$  [Pa]

: gas constant

$V_i$  : Pure Liquid molar volume at temperature, T

: liquid phase mole fraction of component  $i$  [-]

: vapor phase mole fraction of component  $i$  [-]

: Equilibrium Constant or component  $i$

: Temperature, K

### *Subscripts And Superscripts*

:  $i^{\text{th}}$  component

:  $j^{\text{th}}$  Stage (tray)

### *Greek Letters*

: Liquid phase activity coefficient of component  $i$  [-]

: Wilson interaction Parameters

: Liquid molar density

# TABLE OF CONTENTS

<b>Chapter 1 – Introduction</b>	<b>1</b>
1.1 Historical Background	2
1.2 Statement of Problem	3
1.3 Objective of Study	3
1.4 Significance of Study	3
1.5 Scope of Study	3
<b>Chapter 2 – Literature Review</b>	<b>4</b>
2.1 Distillation Categories	4
2.2 Basic Distillation Equipment	8
2.3 General Principles of Distillation	9
2.4 Equilibrium Stage Concept	13
2.5 Thermodynamic Data	14
2.6 Degree Of freedom and design variables	16
2.7 Batch Distillation	18
2.8 Operation Methods	19
2.9 Modelling	21
2.10 Principle Of Formulation	23
2.11 Simulation	23
<b>Chapter Three – Modeling and Simulation</b>	<b>24</b>
3.1 The equations of the model	24
3.2 Model Assumptions	27
3.3 Solution of Modeling Equation	27
3.4 Simulation Algorithm	27
<b>Chapter Four – Data Presentation</b>	<b>28</b>
<b>Chapter Five – Summary, Conclusion and Recommendations</b>	<b>32</b>
5.1 Introduction	32
5.2 Summary	32
5.3 Conclusion	32
5.4 Recommendations	32
<b>Appendix</b>	<b>33</b>
A.1 Vapor pressure using Antoine Equation	33
A.2 Java Simulation of Column	34
<b>References</b>	<b>42</b>



## **CHAPTER ONE**

### **INTRODUCTION**

#### **1.1 BACKGROUND**

Distillation is a process that separates miscible liquids, like alcohol and water. While alcohol can be "boiled out" of the water, some water will also evaporate with the alcohol making the separation incomplete. Therefore, separating two or more liquids requires a bit more technology.

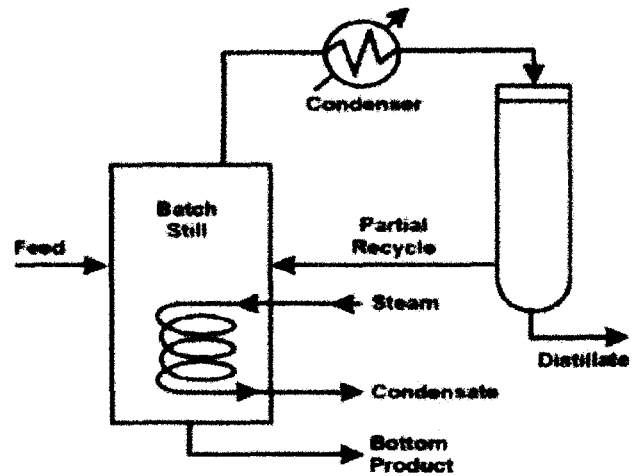
Distillation separates chemicals by the difference in how easily they vaporize. The two major types of classical distillation include continuous distillation and batch distillation. Continuous distillation, as the name says, continuously takes a feed and separates it into two or more products. Batch distillation takes on lot (or batch) at a time of feed and splits it into products by selectively removing the more volatile fractions over time.

Other ways to categorize distillation are by the equipment type (trays, packing), process configuration (distillation, absorption, stripping, azeotropic, extractive, complex), or process type (refining, petrochemical, chemical, gas treating).

Distillation is commonly used in the petroleum industry to separate crude oil into commercial products such as gasoline, jet fuel, Diesel oil, lubricating oils, and asphalt. Many refiners also separate and purify individual compounds (such as propylene). They may also use natural gas as a raw feedstock to make other industrial chemicals such as methanol and then concentrate and purify these using distillation.

Distillation can also be combined with several other processes to produce a desired result. Solvent extraction and distillation may be used to pull a desired chemical from another stream as in the hexane extraction of soy bean oil from soy beans. After the hexane has extracted the oil, it is distilled to purify the oil. The hexane is recycled.

Carbon bed adsorption is also used to recover solvents from dilute air or gas streams. The recovered constituents are then batch distilled.



### 1.1.1 HISTORICAL BACKGROUND

Distillation has been around for a long time. Earliest references are to Maria the Jewess who invented many types of stills and reflux condensers. Common Middle Ages and Renaissance uses of distillation included the manufacture of brandy and other spirits from wine. Another early use was the manufacture of perfumes and essences. Other early users of distillation include the Alchemists. The history of distillation does not end there. Today we use it for more than just spirits.

Many industries use distillation for critical separations in making useful products. These industries include petroleum refining, beverages, chemical processing, petrochemicals, and natural gas processing.

The beverage industry is the one of the oldest users of distillation. Distillation of ethanol for both consumption and other uses was one of the first major industries ever developed.

Natural gas processing started using distillation in the early 1900's. An interesting historical document, Condensation of Gasoline from Natural Gas - <http://www.distillationgroup.com/distillation/H001/H001.htm>, documents some early steps in this industry.

Recent developments energy shortages have re-focused attention on major industrial energy users. Distillation is a major energy consumer. During the energy 'crisis' of the 1970s in the USA much effort was put into making distillation more efficient. A good example of this work is summarized in the Distillation Operations Manual - <http://www.distillationgroup.com/distill.htm#anchor278228> from the Texas Industrial Commission.

Recent developments energy shortages have re-focused attention on major industrial energy users. Distillation is a major energy consumer. During the energy 'crisis' of the 1970s in the USA much effort was put into making distillation more efficient. A good example of this work is summarized in the Distillation Operations Manual – [www.distillationgroup.com/distill.htm#anchor278228](http://www.distillationgroup.com/distill.htm#anchor278228) from the Texas Industrial Institute.

## **2 STATEMENT OF PROBLEM**

The process considered in this process is that of a batch distillation column. The column consists of 8 theoretical stages; a reboiler and the condenser are  $0.015\text{m}^3$  and  $5\text{m}^3$ , respectively. The system consists of a ternary mixture of MTBE, Methanol and Octane. The initial charge, on a molar basis is 25.0% for MTBE, 30.0% for Methanol and 45% for Octane.

## **3 OBJECTIVES OF STUDY**

The goal is to simulate the operation of a batch distillation column based on a rigorous description of the system.

The objective is to use a java program to simulate a batch run

Description of the behaviour of the product quality and the production over time

## **4 SIGNIFICANCE OF STUDY**

The java program can be used for simulation studies and optimization of the operating conditions.

The program can be used to teach students the basics of the operation of a batch distillation column.

## **5 SCOPE OF STUDY**

This study treats the case of a ternary mixture and could be expanded to accommodate other mixtures if appropriate VLE conditions are taken into consideration. The

## CHAPTER TWO

### LITERATURE REVIEW

#### 2.1 DISTILLATION CATEGORIES

Distillation services can be sorted out into many different categories. Here are some basic definitions:

##### 2.1.1 SYSTEM COMPOSITION:

System refers to the chemical components present in the mixture being distilled. The two main groups are *binary distillation* and *multicomponent distillation*.

*Binary distillation* is a separation of only two chemicals. A good example is separating ethyl alcohol (ethanol) from water. Most of the basic distillation teaching and a lot of theoretical work starts with looking at binary distillation; it's a lot simpler.

*Multicomponent distillation* is the separation of a mixture of chemicals. A good example is petroleum refining. Crude oil is a very complex mixture of hydrocarbons with literally thousands of different molecules. Nearly all commercial distillation is multicomponent distillation. The theory and practice of multicomponent distillation can be very complex.

##### 2.1.2 PROCESSING MODE:

Processing mode refers to the way in which feed and product are introduced and withdrawn from the process. Distillation occurs in two modes, *continuous distillation* and *batch distillation*.

*Continuous distillation* is feed is sent to the still all the time and product is drawn out at the same time. That is, continuously takes a feed and separates it into two or more products. The idea in continuous distillation is that the amount going into the still and the amount leaving the still should always equal each other at any given point in time.

*Batch distillation* is when the amount going into the still and the amount going out of the still is not supposed to be the same all the time. Batch distillation takes one batch at a time for the feed and splits it into products by selectively removing the

more volatile fractions over time. The easiest example to use is like old fashioned spirit making. The distiller fills a container at the start, then heats it, as time goes by the vapors are condensed to make the alcoholic drink. When the proper quantity of overhead (drink) is made, the distiller stops the still and empties it out ready for a new batch. This is only a simple case, in industrial usage what goes on gets very complex.

Both continuous and batch distillation are very important to industry. Continuous distillation is most often used with big volume products like jet fuel, benzene, plastic monomers. Batch distillation is most often used with smaller volume products and in plants that make lots of different things and use the same still for many products (in different batches).

### 2.1.3 PROCESSING SEQUENCE:

Fractionation systems have different objectives. The major processing objectives set the system type and the equipment configuration needed. The common objectives include removing a light component from a heavy product, removing a heavy component from a light product, making two products, or making more than two products. We will call these major categories are called *stripping*, *rectification*, *fractionation*, and *complex fractionation*.

This terminology may be a little confusing because we also use the terms *stripping* and *fractionation* when we discuss heat flow options through the unit. This confusion results from historical use of the terms and you just need to keep the context in mind when reading or discussing the material. With a little practice you will find that the reason for using the same terms is that many of the systems called *stripping or fractionation* systems have the same characteristics regardless of using a processing sequence or heat flow analysis of the unit.

***Stripping*** systems remove light material from a heavy product.

***Rectification*** systems remove heavy material from a light product.

***Fractionation*** systems remove a light material from a heavy product and a heavy material from a light product at the same time.

***Complex fractionation*** makes multiple products from either a single tower or a complex of towers combined with recycle streams between them. A good example of a multiple product tower is a refinery crude distillation tower making rough cuts of naphtha (gasoline), kerosene (jet fuel), and diesel from the same tower. A good

example of a complex tower with internal recycle streams is a Petlyck (baffle) tower making three on-specifications products from the same tower.

#### 2.1.4 SYSTEM TYPE:

The behaviour of the chemicals in the system also determines the system configuration for the objectives. The three major problems that limit distillation processes are close-boilers, distributed keys, and azeotropes. Other problems that may require using special system configurations include heat sensitive materials.

*Close boiler* systems include chemicals that boil at temperatures very close to each other. So many stages of distillation or so much reflux may be required that the chemicals cannot be separated economically. A good example is separation of nitro-chloro-benzenes. Up to 600 theoretical separation stages with high reflux may be required to separate different isomers.

*Distributed keys* are systems where some chemicals that we do not want in either the heavy or the light product boil at a temperature between the heavy and the light product.

*Azeotropic* systems are those where the vapor and the liquid reach the same composition at some point in the distillation. No further separation can occur. Ethanol-water is a perfect example. Once ethanol composition reaches 95% (at atmospheric pressure), no further ethanol purification is possible.

Close boilers and distributed keys are economic problems. The compounds can be separated, but it costs a lot. Azeotropic systems are fundamental thermodynamic problems. At the distillation conditions, the products can only be distilled to a certain point, no further.

Different ways to get around these problems include using other techniques (membranes, crystallization, adsorption, adduction, extraction, and precipitation), using complex distillation configurations, changing system conditions, or adding extra chemicals to the process. Adding extra chemicals includes *azeotropic* distillation, *extractive* distillation, or *salt* distillation.

Azeotropic and extractive distillations use the addition of a mass separating agent (MSA) to modify the thermodynamic behaviour of the system. Many different azeotropic and extractive distillation configurations are in use.

**Azeotropic** distillation uses a MSA that forms a minimum boiling azeotrope with some of the feed components is used. The azeotrope is taken overhead and the MSA rich phase decanted and returned to the column as reflux.

**Extractive** distillation uses a MSA that increases the volatility difference between the compounds to be separated. A good example is sulfolane to increase the relative volatility difference between similar molecular weight aromatic and paraffinic hydrocarbons. The sulfolane unit combines liquid-liquid extraction, extractive distillation, and solvent stripping in one process.

**Salt** distillation adds a salt to the system to modify the thermodynamic behaviour of the system. The salt is normally added to the liquid supply of a batch distillation system.

All of these types of systems are normally considered complex systems. Other equipment is needed to separate and reuse the added MSA. Very complex configurations can result. Good understanding of system thermodynamics is required to predict behaviour.

#### 2.1.5 HEAT FLOW:

Energy transfer is required to make separations work. Heat flow refers to the arrangement of the distillation column to its heat source and heat sink. The major categories are *fractionation (distillation)*, *absorption*, *stripping*, and *contacting*.

This terminology may be a little confusing because we also use the terms *stripping* and *fractionation* when we discuss processing sequence options in distillation. This confusion results from historical use of the terms and you just need to keep the context in mind when reading or discussing the material. With a little practice you will find that the reason for using the same terms is that many of the systems called *stripping or fractionation* systems have the same characteristics regardless of using a processing sequence or heat flow analysis of the unit.

**Fractionation** refers to units that have both a reboiler and a condenser. Something is attached to the bottom of the tower to put heat into the tower and something attached to the top of the tower to take heat out of the tower. This is what is normally called distillation

**Absorption** is a unit that has no method at the top of the tower to take heat out. An external stream is supplied from outside the system to absorb material from the vapor.

**Stripping** is a unit that has no method at the bottom of the tower to put heat in. An external stream is supplied from outside the system to strip material from the liquid.

**Contacting** is a unit that has neither a method at the top of the tower to remove heat nor a method at the bottom of the tower to put heat in. Two streams run counter current to each other. Both streams are generated outside the mass-transfer system.

What can make things unclear is that these terms have both other meanings and can be used imprecisely. Also, towers can have intermediate heat input and heat removal equipment in the middle. This confuses the picture. But we will use the strict definitions above. An absorber is a tower without a condenser. A stripper is a tower without a reboiler. A contactor has neither and a fractionator has both.

#### 2.1.6 REACTION:

**Reactive** distillation uses a reaction in the distillation equipment to help the separation. The reaction may or may not use a catalyst. DMT manufacture uses reactive distillation without a catalyst. One process to make methy-tert-butyl-ether uses a catalyst inside the distillation tower. The reaction changes the composition, allowing the distillation to work better.

#### 2.1.7 EQUIPMENT TYPE

Distillation equipment includes two major categories, *trays* and *packing*.

**Trays** force a rising vapor to bubble through a pool of descending liquid.

**Packing** creates a surface for liquid to spread on. The thin liquid film has a high surface area for mass-transfer between the liquid and vapor.

## 2.2 BASIC DISTILLATION EQUIPMENT

Main components of distillation columns

Distillation components are made up of several components, each of which is used either to transfer heat energy or enhance material transfer. A typical distillation contains several major components:

a vertical shell where the separation of liquid components is carried out in column internals such as trays, plates or packings which are used to enhance component separations,

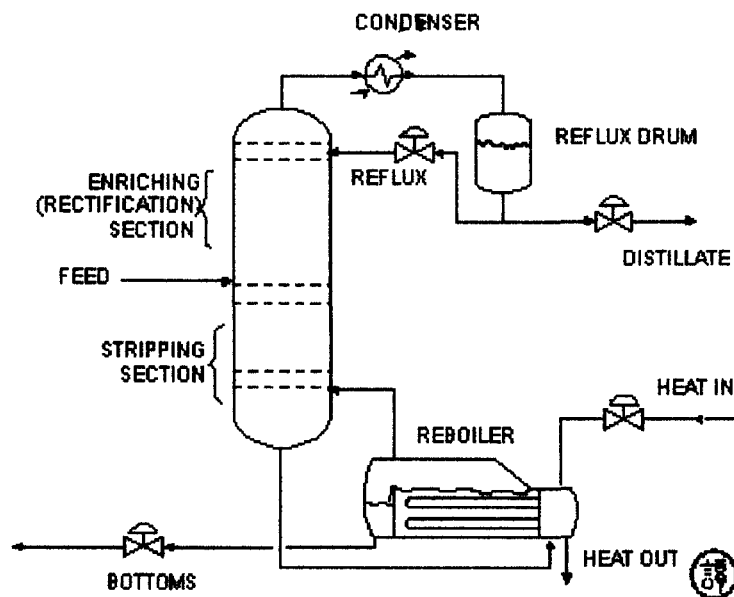
a reboiler to provide the necessary vaporisation for the distillation process,



a condenser to cool and condense the vapor leaving the top of the column,

A reflux drum to hold the condensed vapor from the top of the column so that liquid (reflux) can be recycled back to the column.

The vertical shell houses the column internals and together with the condenser and reboiler, constitutes a distillation column. A schematic of a typical distillation unit with a single feed and two products streams is shown below.



## 2.3 GENERAL PRINCIPLES OF DISTILLATION

Separation of input components, the feed, is achieved by controlling the transfer of components between the various stages (also called trays or plates), within the column, so as to produce output products at the bottom and at the top of the column. In a typical distillation system, two recycle streams are returned to the column. A condenser is added at the top of the column and a fraction of the overhead vapor  $V$  is condensed to form a liquid recycle  $L$ . The liquid recycle provides the liquid stream needed in the tower. The remaining fraction of  $V$ , is the distillate- or top product. A vaporizer or reboiler is added to the bottom of the column and a portion of the bottom liquid,  $L_b$ , is vaporized and recycled to the tower as a vapor stream  $V_b$ . This provides the vapor stream needed in the tower, while the remaining portion of  $L_b$  is the bottom product.

The column consists of  $n$  stages, numbered from top to bottom. The feed enters the column at stage  $n_f$ , with  $1 < n_f < n$ . The feed flow,  $F$  [kmol/hr], is a saturated liquid

with composition  $z_F$  [mole fraction].  $L$  [kmol/hr] denotes the reflux flow rate of the condenser,  $V_b$  [kmol/hr] is the boilup flow rate of the reboiler.

The top product consists of a distillate stream  $D$  [kmol/hr], with composition  $X_d$  [mole fraction]. Likewise, the bottom product consists of a bottom stream  $B$ , with composition  $X_B$  [mole fraction]. The output of the system consists of the distillate composition and bottom composition, respectively.

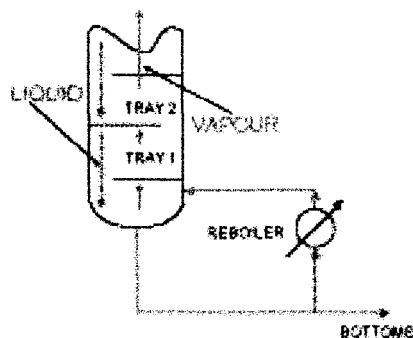
Separation of components from a liquid mixture via distillation depends on the differences in boiling points of the individual components. Also, depending on the concentrations of the components present, the liquid mixture will have different boiling point characteristics. Therefore, distillation processes depends on the vapor pressure characteristics of liquid mixtures.

Separation operations achieve their objectives by the creation of two or more coexisting zones which differ in temperature, pressure, composition and phase state. Each molecular species in the mixture to be separated reacts in a unique way to differing environments offered by these zones. Consequently, as the system moves toward equilibrium each species establishes a different concentration in each zone and this result in a separation between the species.

Separation by distillation utilizes vapour and liquid phases at essentially the same temperature and pressure for the coexisting zones. Various kinds of devices such as random or structured packings and plates or trays are used to bring the two phases into intimate contact. Trays are stacked one above the other and enclosed in a cylindrical shell to form a column. Packings are also generally contained in a cylindrical shell between hold-down and support plates.

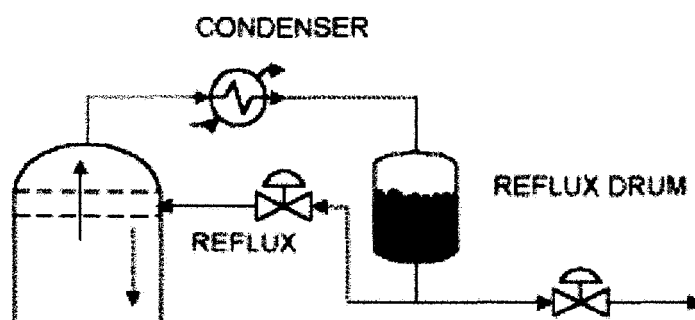
The feed material, which is to be separated into fractions, is introduced at one (or more) point(s) along the column shell. Because of the difference of gravity between vapour and liquid phases, liquid runs down the column, contacting liquid at each tray.

Liquid reaching the bottom of the column is partially vaporized in a heated reboiler to provide boilup, which is sent back up the column.



Heat is supplied to the reboiler to generate vapour. The source of heat input can be any suitable fluid, although in most chemical plants this is normally steam. In refineries, the heating source may be the output streams of other columns. The vapour raised in the reboiler is re-introduced into the unit at the bottom of the column. The remainder of the bottom liquid is removed from the reboiler is known as the bottoms product or simply, bottoms.

The vapour moves up the column, and as it exits the top of the unit, it is cooled by a condenser. The condensed liquid is stored in a holding vessel known as the reflux drum. Some of this liquid is recycled back to the top of the column (this is called the reflux) to provide liquid overflow. The condensed liquid (that is the remainder of the overhead stream) is removed from the system as the distillate or top product. In some cases only part of the vapour is condensed so that a vapour distillate can be withdrawn.



This overall flow pattern in a distillation column provides counter-current contacting of vapour and liquid streams on all trays through the column. Vapour and liquid phases on a given tray approach thermal, pressure and composition to an exact extent dependent upon the efficiency of the contacting tray.

The lighter (lower boiling) components tend to concentrate in the vapour phase, while the heavier (higher-boiling) components tend toward the liquid phase. The result is a vapour phase that becomes richer in light components as it passes up the column and a liquid phase that becomes richer in heavy components as it cascades downward. The overall separation achieved between the distillate and the bottoms depends primarily on the relative volatilities of the components, the number of contacting trays, and the ratio of the liquid-phase flow rate to the vapour-phase flowrate.

If the feed is introduced at one point along the column shell, the column is divided into an upper section, which is often called the *Rectifying section* and a lower section, which is often referred to as the *Stripping section*. These terms become rather indefinite in multiple – feed columns and in columns from which a liquid or vapour side stream is withdrawn somewhere along the column length in addition to the two end product streams.

## 2.4 EQUILIBRIUM STAGE CONCEPT

In the past, energy and mass transfer processes in an actual distillation column were considered too complicated to be readily modelled in any direct way. This difficulty was circumvented by the equilibrium stage model, developed by Sorel in 1893 in which vapour and liquid streams leaving an equilibrium stage are in complete equilibrium with each other and thermodynamics relations can be used to determine the temperature of and relate the concentrations in the equilibrium streams at a given pressure. A hypothetical column composed of equilibrium stages (instead of actual trays) is designed to accomplish the separation specified for the actual column. The number of hypothetical equilibrium stages is then converted to a number of actual trays by means of *tray efficiencies*, which describe the extent to which the performance of an actual contact tray duplicates the performance of an equilibrium stage. Alternatively and preferably, tray efficiencies can be accounted for by using *rate-based* models that are described below.

Use of the equilibrium-stage concept separates the design of a distillation column into three major steps:

Thermodynamic data and methods needed to predict equilibrium-phase compositions are assembled.

The number of equilibrium stages required to accomplish a specified separation, or the separation that will be accomplished in a given number of equilibrium stages, is calculated.

The number of equilibrium stages is converted to an equivalent number of actual contact trays or height of packing and the column diameter is determined.

## 2.5 THERMODYNAMIC DATA

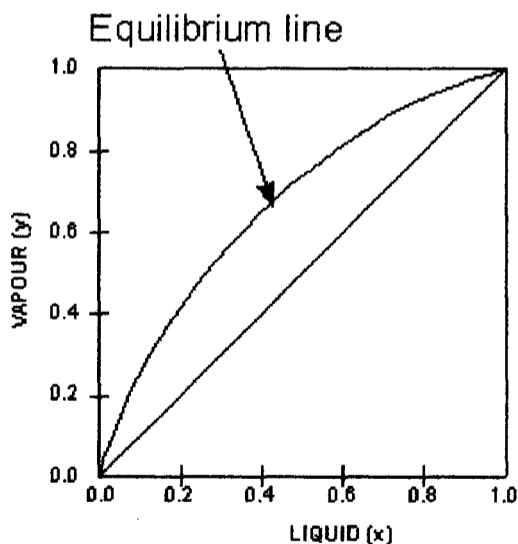
Reliable thermodynamic data are essential for the accurate design or analysis of a distillation column. Failure of equipment to perform at specified levels is often attributable, at least in part, to the lack of such data.

### 2.5.1 PHASE EQUILIBRIUM DATA

Distillation columns are designed based on the boiling point properties of the components in the mixtures being separated.

For a binary mixture, pressure and temperature fix the equilibrium vapor and liquid compositions. Experimental data are frequently presented in the form of tables of vapor mole fraction  $y$  and liquid mole fraction  $x$  for one constituent over a range of temperature  $T$  for a fixed pressure  $P$  or over a range of pressure for a fixed temperature.

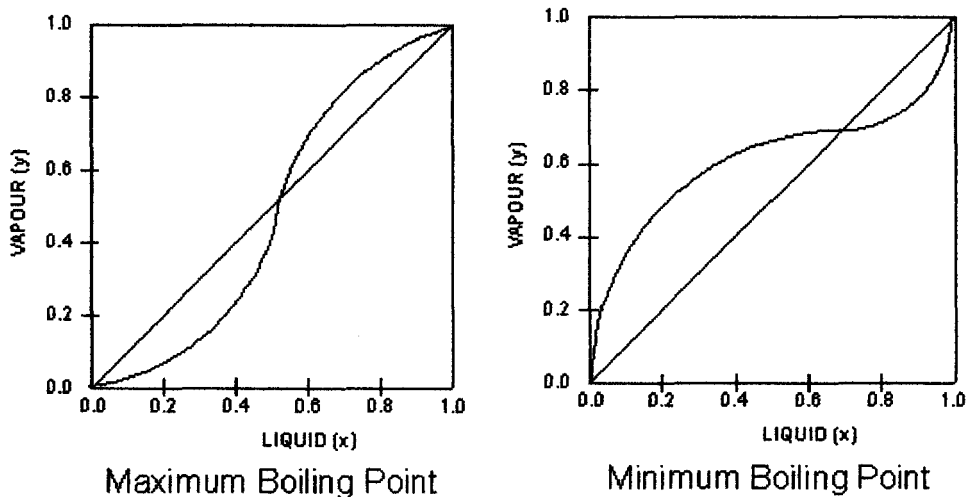
For application to distillation, binary mixture data are frequently plotted for a fixed pressure, as  $y$  versus  $x$ , with a line of  $45^\circ$  slope included for reference, and as  $T$  versus  $y$  or  $x$ . The sizes, particularly the height, of distillation columns are determined by the vapour liquid equilibrium (VLE) data for the mixtures. The VLE plot expresses the bubble-point and the dew-point of a binary mixture at constant pressure. The curved line is called the equilibrium line and describes the compositions of the liquid and vapour in equilibrium at some fixed pressure.



In most binary systems, one of the components is more volatile than the other over the entire composition range. This is the case in a benzene-toluene system at

pressures of 101.3 and 202.6 *kPa* (i.e. 1 and 2 *atm*) where benzene is more volatile than toluene.

For some binary systems, one of the components is more volatile only a part of the composition range. For example ethyl acetate-ethanol and chloroform-acetone. Such mixtures are known as Azeotropic mixtures and the composition in which vapor and liquid compositions are equal, is the azeotropic composition or *azeotrope*. The most intriguing VLE curves are generated by azeotropic systems:



Non azeotrope forming mixtures such as benzene and toluene can be separated by simple distillation into two essentially pure products. By contrast, simple distillation of an azeotropic mixture will at best yield the azeotrope and one essentially pure species.

For mixtures containing more than two species, an additional degree of freedom is available for each additional component e.g. for a four component system, the equilibrium vapor and liquid compositions are only fixed if the pressure, temperature and mole fractions of two components are set.

Representation of multicomponent vapor-liquid equilibrium data in tabular or graphical form of the type obtained for binary systems is either difficult or impossible. Instead such data, as well as binary system data are commonly represented in terms of *K* values (vapor-liquid equilibrium ratios), which is defined by

$$K_i = \frac{y_i}{x_i}$$

and are correlated empirically or theoretically in terms of temperature, pressure and phase compositions in form of tables, graphs and equations.  $K$  values are widely used in multi component distillation calculations and the ratio of the  $K$  values of two species called the *relative volatility*,

$$\alpha_{ij} = \frac{K_i}{K_j}$$

is a convenient index of the relative ease or difficulty of separating components  $i$  and  $j$  by distillation. Relative volatility is a measure of the differences in volatility between 2 components, and hence their boiling points. Thus if the relative volatility between 2 components is very close to one, it is an indication that they have very similar vapour pressure characteristics. This means that they have very similar boiling points and therefore, it will be difficult to separate the two components via distillation.

## 2.6 DEGREE OF FREEDOM AND DESIGN VARIABLES

### 2.6.1 DEFINITIONS

For separation processes, a design solution is possible if the number of independent equations equals the number of unknowns.

$$N_i = N_v - N_c$$

$N_v$  = Total No. of variables (unknowns)

$N_c$  = No. of restricting relationships among the unknowns

$N_i$  = No. of design variables

In the analogous phase rule analysis,  $N_i$  is usually referred to as the degree of freedom or variance. It is the no. of variables that the designer must specify to define one unique operation (solution) of the process.

The variable  $N_i$  with which to be concerned are:

Stream concentrations (e.g. Mole fractions)

temperatures

Pressures

Stream Flow Rates

Repetition variables  $N_r$

The first three are intensive variables. The fourth is an extensive variable that is not considered in the usual phase rule analysis. The fifth is neither an intensive nor an



extensive variable but is a single degree of freedom that the designer utilizes in specifying how often a particular element is repeated in a unit.

The various restricting relationships  $N_c$  can be classified as

Inherent

Mass-balance

Energy-balance

Phase Distribution

Chemical Equilibrium

Inherent restrictions are usually the result of definitions and take the form of identities. The concept of equilibrium stage involves the inherent restrictions that

$$T^V = T^L; P^V = P^L$$

Mass balance restrictions are the  $n$  balances written for the  $n$  components present in the system. An alternative is to write  $(n - 1)$  component balances and one overall mass balance.

The phase distribution restrictions reflect the requirement that  $f_i^V = f_i^L$  at equilibrium where  $f$  is the fugacity. When all the components exist in all phases, the number of restricting relationships due to the distribution phenomenon will be  $n(N_p - 1)$ , where  $N_p$  is the number of the phase present.

For distillation analysis, the forms in which the restricting relationships are expressed are unimportant. Only the number of such restrictions is important. A degrees of freedom analysis must be made before unit operations can be successfully modelled with a process simulator.

### 2.6.2 FIXED VARIABLES

Existing distillation columns such as in Unit Operations Laboratory have variables that are fixed that we cannot manipulate to alter the output. These variables are for instance: the height of the column, the number of trays, the plate efficiency, the tray hold-ups, the material of the tower, the thickness of the walls and so on.

### 2.6.3 INDEPENDENT VARIABLES

On the other hand there are a number of variables that can be controlled so the column output can be varied depending on the objective:

Feed  $F$  (that is feed temperature and pressure as well as feed concentrations and mass flowrate)

Steam flowrate and conditions (thus the reboiler duty  $Q_r$  in the simulation).

Reflux ratio  $R$

Feed plate location

These variables are the ones that are available for planning experiments on the distillation columns.

#### 2.6.4 DEPENDENT VARIABLES

With the fixed and independent variables defined for the column, we can now solve for not only the exit concentrations at the top and the bottom of the column but also all variables in the column. Any of these independent variables can be manipulated (adjusted) to either maximize or minimize the product component concentrations.

### 2.7 BATCH DISTILLATION

Batch distillation is versatile and has many advantages. It is the method of choice in the following situations:

when small amounts of a material are needed

when a plant does not run continuously

when distillation is required only occasionally

when the same equipment can be used to separate different mixtures

when separating more than one component from a solution with one equipment set-up.

The disadvantages of batch distillation are that only one pure product is removed and the process is not operated at steady state.

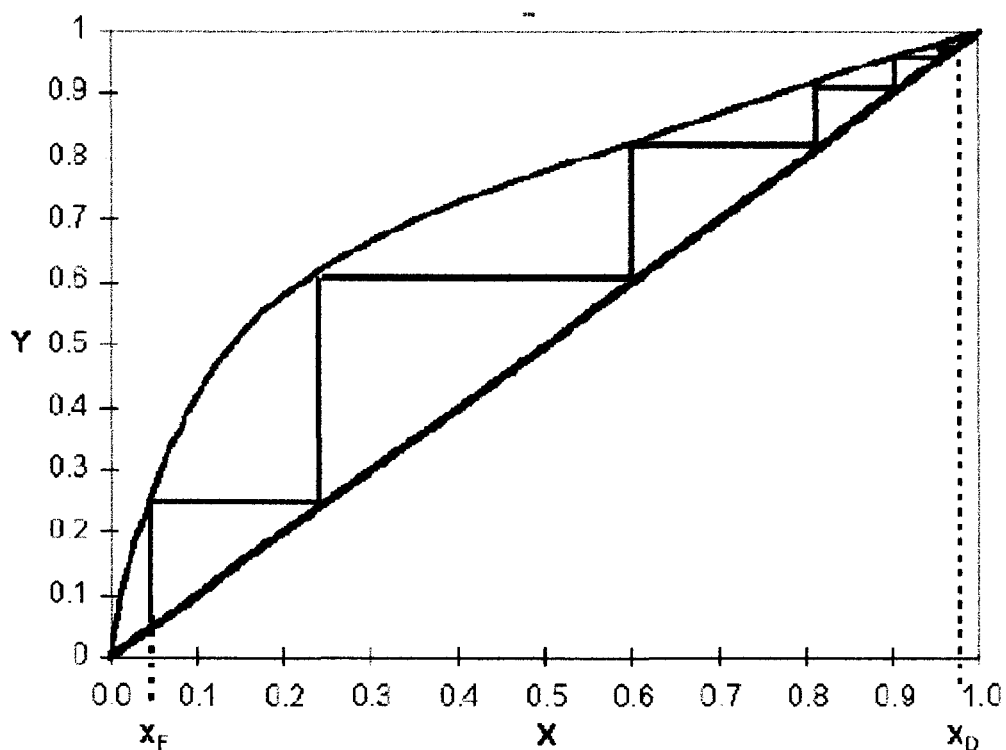
In batch distillation, the mixture to be separated is charged to a still pot and heated. As vapors form, they rise up the column becoming enriched in the more volatile component. A column contains trays that allow for liquid-vapor contact. Sieves, valves, and bubble caps are different types of trays used in columns. The vapor bubbles through these slots while the liquid flows across the tray. Another opening surrounded by a weir is located at one end of the tray. The weir acts as a dam and allows liquid to flow over it to drop to the plate below. The vapors from the top stage

are condensed and can be recovered as product or returned to the column. Progress of a batch distillation can be monitored by measuring stage temperatures. Each stage is at its bubble point, and the stage temperature is therefore theoretically a measure of stage composition. Samples of liquid can be obtained from each tray. The higher the number of stages, the better the separation which can be obtained. Three different operations are possible for batch distillation: total reflux ratio, constant reflux ratio, and constant distillate composition.

## 2.8 OPERATION METHODS

### 2.8.1 TOTAL REFLUX

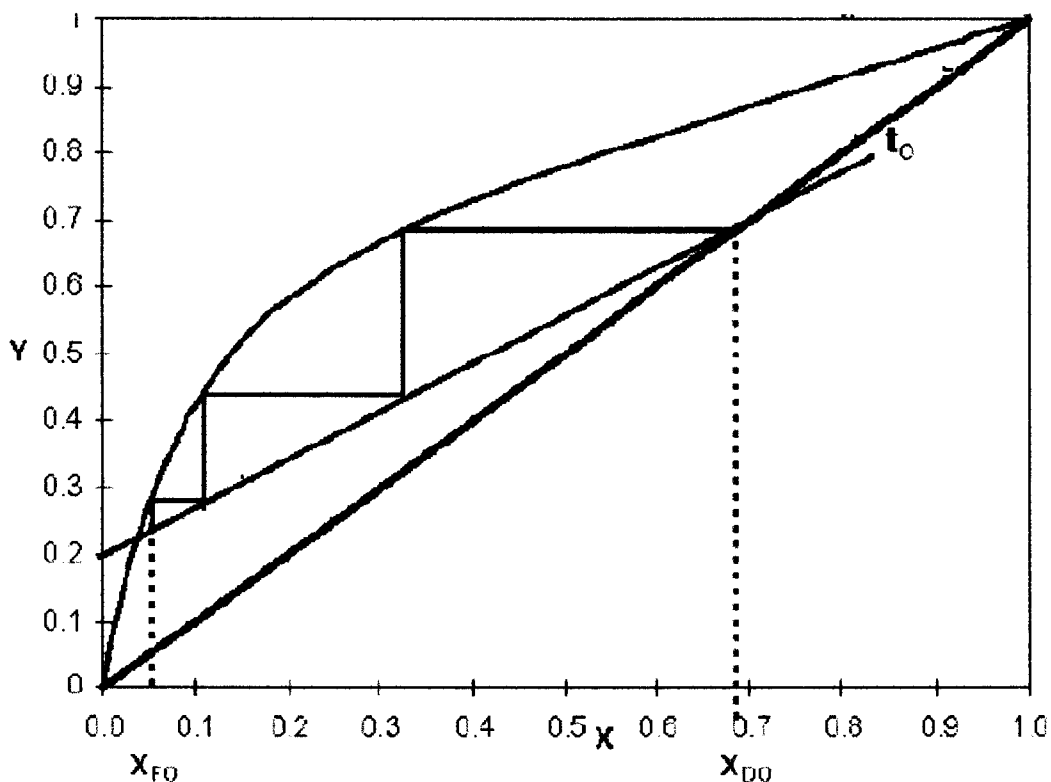
Batch distillation operated at total reflux returns all the condensed vapors to the column. Steady-state is reached as no product is removed. Operating a column at total reflux is a convenient method of studying the performance of the column because compositions will not change with time. Simple equations relate flow rates and compositions. Because the stages are at steady state, the flow rates of passing streams must be equal. Therefore the composition and the flow rate of the rising vapor from one tray must be equal to the composition and flow rate of the liquid descending from the tray above. In this way, vapor compositions can be obtained from liquid samples. A McCabe-Thiele diagram for total reflux ratio uses the  $X=Y$  line as the operating line, and the feed and distillate compositions remain constant.

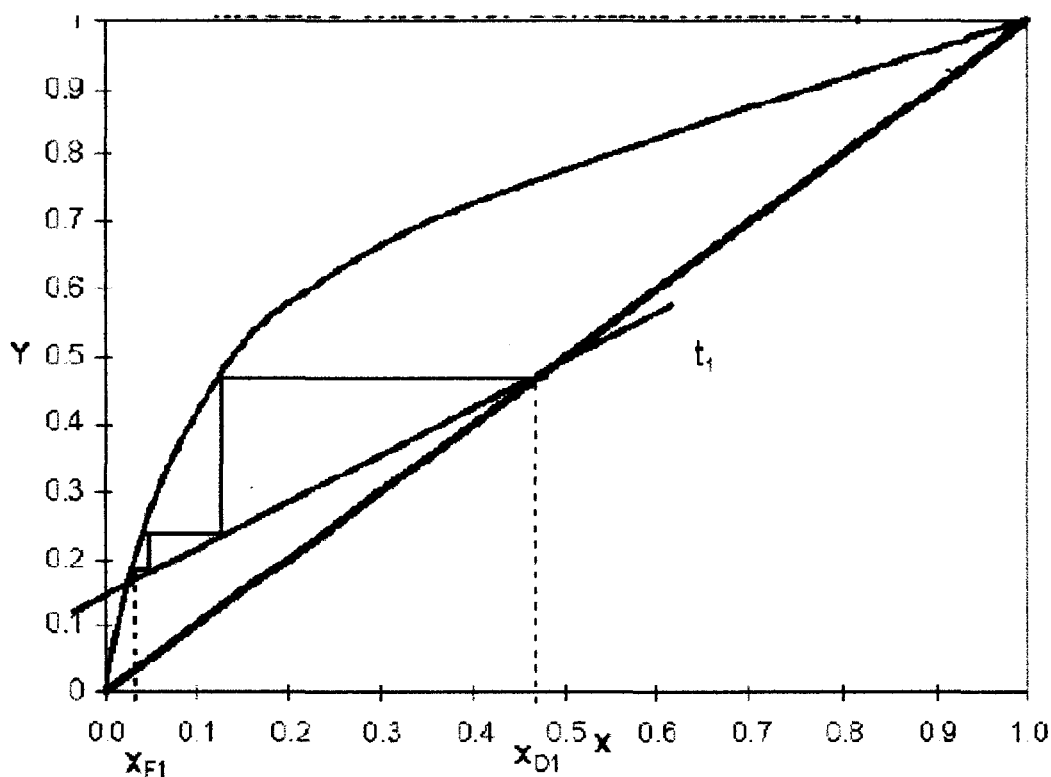


## McCabe Thiele Diagram at total Reflux

## 2.8.2 CONSTANT REFLUX RATIO

The reflux ratio is the ratio of the liquid returning to the column to the distillate removed. Batch distillation operated at a constant reflux ratio is an unsteady state process. The composition in the still pot and the stages continually changes as product is removed. The vapors from the top stage are condensed and some of the condensate is returned to the column as reflux; the remainder is collected as product. The composition of the distillate being collected also changes with time. A McCabe-Thiele diagram for constant reflux ratio relates the composition of the distillate to the composition of the feed remaining in the reboiler at any time for a column with 100% tray efficiency. The operating line has a constant slope because the slope is a function of the reflux ratio and is shifted for varying feed conditions to find the resulting distillate composition. The Figures below show the McCabe-Thiele diagrams for a column with 100% efficiency at times  $t_0$  and  $t_1$  respectively. In commercial practice, high reflux ratios are undesirable because of heating and cooling costs. Thus, the column is operated at the lowest reflux ratio possible for the separation desired.

McCabe-Thiele diagram for constant reflux at an early time  $t_0$ .



McCabe-Thiele diagram for constant reflux at a later time  $t_1$ .

### 2.8.3 CONSTANT DISTILLATE COMPOSITION (VARYING REFLUX)

Using batch distillation to collect a constant composition distillate product requires varying the reflux ratio as the distillation progresses. Lower reflux ratios are used when the separation is easier, and higher reflux ratios are needed when the separation becomes more difficult. On a McCabe-Thiele diagram for varying reflux ratios the operating line intersects the  $X=Y$  line at the distillate composition. The slope of the operating line now varies with feed composition, but the distillate composition remains constant. This is a difficult process to control without extensive instrumentation.

## 2.9 MODELING

Definition of a model:

A simplified or idealized description of a system, situation, or process, often in terms, devised to facilitate calculations and predictions.

A representation of an object, system or idea in a form other than that of the entity/system itself.

An abstraction and simplification of the real world.

A mathematical model is a numerical time advance representation of some real world system. Modeling is a powerful tool that is often applied to the design and

analysis of complex systems. Decisions can be made about the system by constructing computer models of it and conducting experiments on the model.

### 2.9.1 CLASSIFICATION OF MODELS

Models fall into the following categories:

**Analytical/Mathematical models.** These are mathematical equations. Representing a system in terms of quantitative relationships. These models often describe forces that exist between objects. The purpose of such models is often to investigate what impact there will be on the system as a whole if changes are made to individual elements of the system.

**Visual models.** These are graphical representations. Examples are schematic diagrams of electronic equipment or flow charts that describe the logic of a computer program. The purpose of these models is usually to enable the operating rules and processes of a system to be understood.

**Physical models.** These are physical models usually at a reduced scale.

In very simple terms a model is a description of a real life system and the form that the model takes is very dependent on the purpose of the model.

### 2.9.2 SYSTEM MODELING - FUNCTIONS OF MODELS

As an analytical tool

Analyze manufacturing systems

Evaluating equipment requirements

Design of transport facility

As an aid for experimentation

For planning and scheduling

There are a number of reasons why it may be preferable to carry out experiments on a model rather than directly on the real system:

The results of the experiment may be unpredictable or dangerous to the system or the personnel operating it.

Experiments may unacceptably disrupt the operational requirements of the system.

A new system may require design decisions to be made prior to construction of the system.

A simulation experiment may be precisely repeated any number of times. In many instances a real dynamic system would not allow precise replication.

Confidentiality is easier to maintain with a computer simulation where only a few key people would be privy to the results. The results of experimenting with a real system are more open.

Time scale of the real system may be too long, or too short for convenient experimentation.

Training.

## 2.10 PRINCIPLES OF FORMULATION

**2.10.1 BASIS.** The bases of mathematical models are the fundamental physical and chemical laws, such as the laws of conservation of mass, energy, and momentum.

**2.10.2 ASSUMPTIONS.** An extremely rigorous model that includes every phenomenon down to microscopic detail would take a long time to develop and might be impractical to solve. An engineering compromise between the rigorous description and getting an answer that is good enough is always required when modeling. So the engineer has to use his discretion(judgment) to make reasonable valid assumptions.

**2.10.3 MODELING ALGORITHM.** Available solution techniques and tools should be kept in mind as a mathematical model is developed.

## CHAPTER THREE

### MODELING AND OPTIMIZATION

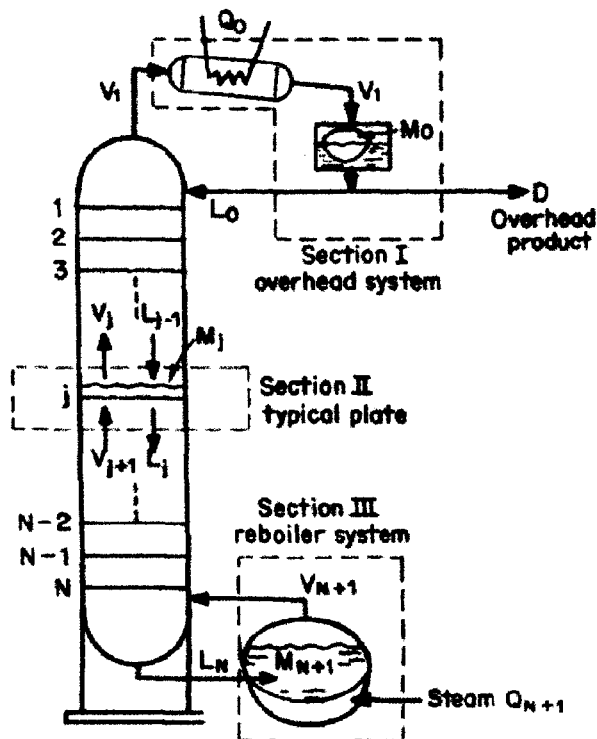


Figure 3.1: Schematic of a batch-distillation column.

### 3.1 THE EQUATIONS OF THE MODEL

The batch distillation column can be modelled by combining the mass balance equation with thermodynamic equilibrium data as follows. The goal is to relate the composition and amount of the distillate and the remaining feed to the VLE relationship. System balances are as follows:

The Component mole balance reads:

Total-condenser-reflux drum:

$$\frac{dx_{i,0}}{dt} = - \left[ \frac{L_0 + D + \frac{dM_0}{dt}}{M_0} \right] x_{i,0} + \left[ \frac{V_i K_{i,1}}{M_0} \right] x_{i,1} \quad (3.1)$$

Trays:

$$\frac{dx_{i,j}}{dt} = \left( \frac{L_{j-1}}{M_j} \right) x_{i,j-1} - \left[ \frac{L_j + K_{i,j} + \frac{dM_j}{dt}}{M_j} \right] x_{i,j} + \left[ \frac{K_{i,j} V_{j+1}}{M_j} \right] x_{i,j+1} \quad (3.2)$$

Reboiler:



$$\frac{dx_{i,N+1}}{dt} = \left( \frac{L_N}{M_{N+1}} \right) x_{i,N} - \left[ \frac{V_{N+1} K_{i,N+1} + \frac{dM_{N+1}}{dt}}{M_{N+1}} \right] x_{i,N+1} \quad (3.3)$$

where  $i = 1$  to  $C$ ,  $j = 1$  to  $N$  &  $L_0 = RD$

Total mole balance reads:

Total-condenser-reflux drum:

$$V_1 = D(R-1) + \frac{dM_0}{dt} \quad (3.4)$$

Trays:

$$L_j = V_{j+1} + L_{j-1} - V_j - \frac{dM_j}{dt} \quad j = 1 \text{ to } N \quad (3.5)$$

Molar hold-ups:

$$\text{Condenser-Reflux Drum:} \quad M_0 = G_0 \rho_0 \quad (3.6)$$

$$\text{Trays:} \quad M_j = G_j \rho_j \quad j = 1 \text{ to } N \quad (3.7)$$

$$\text{Reboiler:} \quad M_{N+1} = M_{N+1}^0 - \sum_{j=0}^N M_j - \int_0^t D dt \quad (3.8)$$

Energy balance around jth tray:

$$V_{j+1} = \frac{1}{(H_{V_{j+1}} - H_{L_j})} \left[ V_j (H_{V_j} - H_{L_j}) - L_{j-1} (H_{L_{j-1}} - H_{L_j}) + M_j \frac{dH_{L_j}}{dt} \right] \quad (3.8b)$$

$j = 2$  to  $N + 1$

The above is merely mass and energy balances; thermodynamic information (i.e. the VLE relationship) has not yet been used. That is done below:

$P_i^{sat}$  is the vapor pressure of pure component  $i$  and is calculated by using Antoine equation of which constants are listed in *Appendix A*.

$$\ln P_i^{sat} = A_i - \frac{B_i}{T + C_i} \quad (3.9)$$

So that,

$$P_i^{sat} = e^{\left( A_i - \frac{B_i}{T + C_i} \right)} \quad (3.10)$$

Based on equation 3.1,  $x$ - $y$  relation can be predicted by using activity coefficients.

The Wilson equation is a very useful equation:

$$\ln \gamma_i = 1 - \ln \sum_j x_j \Lambda_{ij} - \sum_k \frac{x_k \Lambda_{ki}}{\sum_j x_j \Lambda_{kj}} \quad (3.11)$$

So that,

$$\gamma_i = e^{\left(1 - \ln \sum_j x_j \Lambda_{ij} - \sum_k \frac{x_k \Lambda_{ki}}{\sum_j x_j \Lambda_{kj}}\right)} \quad (3.12)$$

where  $A_{ij} = 1$  for  $i = j$  and  $A_{ij} \neq A_{ji}$ .

Temperature dependence on the parameter is given as:

$$A_{ij} = \frac{V_j}{V_i} e^{\frac{-\Lambda_{ij}}{RT}} \quad (3.13)$$

The Modified Raoult's Law K value equation is then applied to give the equilibrium constants for components  $i$ ,

$$K_i = \frac{\gamma_i P_i^{sat}}{P} \quad (3.14)$$

VLE relation can then be expressed by the following equation when no significant interaction occurs in the vapor phase:

$$y_i = x_i \frac{\gamma_i P_i^{sat}}{P} \quad (3.15)$$

Temperature per stage in the Batch column is obtained by:

$$T_i = \frac{P - \gamma_1 P_1^{sat} x_1 - \gamma_2 P_2^{sat} x_2 - \gamma_3 P_3^{sat} x_3}{P} \quad (3.16)$$

### 3.2 MODEL ASSUMPTIONS

The model for the batch distillation column has been developed using a number of model assumptions. The model assumptions are listed below:

The liquid and the vapor leaving a stage are in thermodynamic equilibrium.

Total condensation with no sub-cooling in the condenser.

No entrainment and weeping effects.

Constant tray efficiency

Adiabatic operation

Phase equilibrium

Perfect mixing on trays and in the reboiler drum

Non-ideal vapour phase.

### 3.3 SOLUTION OF MODEL EQUATIONS

There are several numerical methods that can be employed to integrate the model differential equations and solve the algebraic ones. They include Newton Raphson method, Runge-kutta method, Euler method and so on. The fourth-order Runge-Kutta method will be employed to solve the differential equations in this project. The fourth-order Runge-Kutta algorithm is one of the best all-round algorithms that has been developed and is probably the most widely used numerical scheme. It has a small truncation error.

### 3.5 PROGRAM DESCRIPTION

1. The program is started by going to the start menu, point at programs then select Batch Simulation. Then click on the program icon to launch the program.
2. As soon as the program loads successfully the user is prompted to enter mixture parameters such as component names. For example, I key in the components of my mixture as MTBE, Methanol and Octane and then click okay.
3. The program then searches the database that contains the Antoine's constants to see if all mixture parameters are available in the database. If the parameters are available it displays them for the user to confirm that they are correct. The parameters displayed include Antoine's constants A, B, C, boiling temperature of component. After confirming that the parameters displayed are correct the user should click the ok button to proceed.
4. The program then requests for the composition of the mixture to be introduced into the reboiler of the distillation column. For example, 10% Methanol, 50% Chloroform and 40% Acetone.
5. The program then requests the number of trays in the existing column to be simulated, molar hold-up on the trays and in the condenser and initialization conditions for the column. For example say I were to simulate an 8 tray column and to initialize the reboiler at 70°C, with molar hold-up on the tray as 0.015m<sup>3</sup> and in condenser as 0.005m<sup>3</sup>.
6. The program requests for the reflux ratio, boilup rate for distillate withdrawal.
7. With the information provided, the program simulates and predicts the total-reflux conditions of the column. Then it predicts the withdrawal conditions for withdrawal of the first component from the column, it does the same thing for the next component. The final component should be withdrawn from the reboiler.

## CHAPTER 4

### DATA PRESENTATION AND DISCUSSION

Initially the program simulates the total-reflux conditions of the batch distillation column predicting stage temperatures at 336.3 K in the reboiler to about 326.5 K in the condenser. The simulation gives a composition of 0.308 for MTBE, 0.622 for Methanol and 0.070 for Octane in the condenser at steady state operation of the distillation column.

The program then simulates the withdrawal of the component with the lowest boiling point in the mixture which is MTBE. My simulation predicts the withdrawal of MTBE at 328.0 K which is approximately the boiling point of MTBE. At this temperature the purity of MTBE is 95.2%.

A second step of the distillation column is simulated the withdrawal of methanol from the still. This occurs at 334.1 K which is approximately the boiling point of methanol. The third and final product is withdrawn from the reboiler.

The model successfully predicts the product quality and production of a batch distillation column. Presented below are the predicted column compositions. The first table shows the steady state reflux calculation for the column. The second table presents the conditions at the withdrawal of MTBE from the column; and the third table presents the conditions at the withdrawal of methanol from the column. The third and final product (acetone) is withdrawn from the reboiler. The table below shows the temperature, liquid composition, vapour composition and the liquid phase activity coefficient of component from stage to stage denoted as  $x_1, x_2, x_3, y_1, y_2, y_3, \gamma_1, \gamma_2, \gamma_3$  respectively. Where MTBE is component 1, Methanol is component 2, Octane is component 3.

The simulation of the column based on the rigorous description of the system has been successful. The program performed within expected limits.

	T[K]	x1	x2	x3	y1	y1	y3	Gamma 1	Gamma 2	Gamma 3
<b>Reboiler</b>	336.3	0.243	0.283	0.474	0.620	0.313	0.067	1.029	5.543	1.191
<b>Stage 11</b>	332.9	0.222	0.253	0.525	0.564	0.380	0.056	1.017	4.354	1.309
<b>Stage 10</b>	332.0	0.443	0.150	0.07	0.504	0.443	0.053	1.005	3.711	1.339
<b>Stage 9</b>	329.9	0.210	0.651	0.139	0.340	0.613	0.047	1.531	1.290	3.787
<b>Stage 8</b>	328.7	0.700	0.161	0.139	0.691	0.291	0.018	0.970	2.611	1.525
<b>Stage 7</b>	328.7	0.412	0.314	0.274	0.510	0.449	0.041	1.215	2.062	1.775
<b>Stage 6</b>	328.2	0.256	0.668	0.076	0.408	0.564	0.028	1.588	1.243	4.554
<b>Stage 5</b>	328.0	0.952	0.023	0.025	0.943	0.054	0.003	0.995	3.535	1.414
<b>Stage 4</b>	327.2	0.712	0.200	0.088	0.693	0.295	0.012	1.005	2.265	1.639
<b>Stage 3</b>	327.1	0.295	0.636	0.069	0.419	0.559	0.022	1.472	1.356	4.028
<b>Stage 2</b>	327.0	0.794	0.102	0.104	0.785	0.197	0.018	1.034	3.013	2.318
<b>Stage 1</b>	326.8	0.433	0.500	0.067	0.498	0.487	0.015	1.212	1.542	3.020
<b>Condenser</b>	326.5	0.308	0.622	0.070	0.451	0.532	0.017	1.547	1.353	3.141

Table 4.1 Total Reflux Conditions

	T[K]	x1	x2	x3	y1	y1	y3	Gamma 1	Gamma 2	Gamma 3
<b>Reboiler</b>	334.6	0.327	0.111	0.562	0.402	0.519	0.079	1.001	5.277	1.283
<b>Stage 11</b>	334.3	0.301	0.055	0.644	0.456	0.434	0.110	1.248	9.100	1.575
<b>Stage 10</b>	333.9	0.324	0.236	0.440	0.370	0.565	0.065	0.949	2.782	1.392
<b>Stage 9</b>	333.4	0.279	0.224	0.497	0.338	0.592	0.070	1.024	3.142	1.355
<b>Stage 8</b>	332.9	0.272	0.302	0.426	0.330	0.605	0.065	1.040	2.430	1.510
<b>Stage 7</b>	332.8	0.311	0.273	0.416	0.349	0.586	0.065	0.967	2.607	1.552
<b>Stage 6</b>	332.4	0.373	0.153	0.474	0.431	0.500	0.069	1.010	4.040	1.455
<b>Stage 5</b>	332.0	0.271	0.373	0.356	0.321	0.619	0.060	1.046	2.084	1.735
<b>Stage 4</b>	330.8	0.309	0.439	0.252	0.379	0.571	0.050	1.126	1.716	2.126
<b>Stage 3</b>	329.9	0.337	0.322	0.341	0.370	0.577	0.053	1.037	2.456	1.753
<b>Stage 2</b>	329.7	0.391	0.328	0.281	0.453	0.502	0.045	1.103	2.117	1.811
<b>Stage 1</b>	329.1	0.332	0.350	0.318	0.395	0.551	0.054	1.153	2.229	1.983
<b>Condenser</b>	328.0	0.952	0.023	0.025	0.943	0.054	0.003	0.995	3.535	1.414

Table 4.2 Conditions At Withdrawal of MTBE

	T[K]	x1	x2	x3	y1	y1	y3	Gamma 1	Gamma 2	Gamma 3
Reboiler	344.5	0.436	0.009	0.555	0.794	0.095	0.111	1.099	8.631	1.211
Stage 10	342.4	0.490	0.010	0.500	0.813	0.101	0.086	1.067	8.174	1.135
Reboiler	342.2	0.487	0.006	0.507	0.845	0.070	0.085	1.123	10.108	1.118
Stage 8	340.5	0.519	0.015	0.466	0.812	0.108	0.080	1.064	6.678	1.220
Stage 7	338.9	0.191	0.091	0.718	0.253	0.637	0.110	0.944	6.650	1.169
Stage 6	338.2	0.559	0.017	0.424	0.817	0.113	0.070	1.066	6.489	1.308
Stage 5	336.3	0.466	0.060	0.474	0.620	0.313	0.067	1.029	5.543	1.191
Stage 4	335.7	0.242	0.154	0.604	0.290	0.624	0.086	0.944	4.390	1.241
Stage 3	334.6	0.151	0.401	0.448	0.183	0.743	0.074	0.983	2.099	1.510
Stage 2	334.6	0.327	0.111	0.562	0.402	0.519	0.079	1.001	5.277	1.283
Stage 1	334.3	0.434	0.088	0.478	0.535	0.400	0.065	1.013	5.185	1.259
Condenser	334.1	0.077	0.735	0.188	0.138	0.779	0.083	1.491	1.224	4.063

Table 4.3: Conditions after Withdrawal of Methanol



## CHAPTER FIVE

### CONCLUSION AND RECOMMENDATIONS

#### 5.1 CONCLUSION

In this work, the case of Methyl Tertiary Butyl Ether – Methanol – Octane mixture was considered to test the capability of the modelling equations and the java program. The process was successfully simulated and the model performed within acceptable limits in describing the vapour and liquid composition of the column from tray to tray. The model also predicted the tray temperatures of the column.

A java program predicting the batch simulation for the ternary mixture (Methyl Tertiary Butyl Ether – Methanol – Octane) batch distillation has been developed by employing a rigorous process description of a typical batch column. The program successfully predicted the process behaviour and described the behaviour of the column over time from stage to stage.

#### 5.2 RECOMMENDATIONS

The model could be more detailed, for example by using tray efficiencies that vary over time. Of course this would make the simulation more difficult but it would end up developing a more reliable model that can predict batch column behavior over time which will be much more accurate.

## APPENDIX

### A.1 VAPOR PRESSURE USING ANTOINE EQUATION

The pure component vapour pressures,  $P^{sat}$  were derived from the Antoine equation (Antoine, 1888).

$$\ln P^{sat} = A - \frac{B}{T + C}$$

Where A, B, C are constants for a given Species.

In this case,

Component 1: Methyl Tertiary Butyl Ether

Component 2: Methanol

Component 3: Octane

Component i	A	B	C	Boiling Point(K)
1	6.038757	1149.261	-43.150	328.3
2	7.025886	1474.078	-44.020	337.7
3	6.043940	1351.938	-64.030	398.9

### BINARY INTERACTION PARAMETERS AND ACTIVITIES FOR WILSON MODEL

$$A_{12} = 0.5004$$

$$A_{13} = 2.0778$$

$$A_{23} = 0.09749$$

$$A_{21} = 0.4804$$

$$A_{31} = 0.2115$$

$$A_{32} = 0.05240$$

## A.2 SIMULATION INTERFACE

Stage	T	M	x1	x2	x3	y1	y2	y3
Condenser	0.998	0.01	0.1	0.1	0.1	0.715	0.246	0.039
Stage 1	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 2	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 3	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 4	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 5	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 6	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 7	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 8	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Reboiler	0.987	100	0.323	0.224	0.453	0.298	0.677	0.024

## A.3 JAVA CODE FOR COLUMN SIMULATION

```

/*
 * Input.java
 * */

//package Model;

import java.lang.Math.*;
import java.awt.*;
import javax.swing.*;
import javax.swing.border.*;
import java.awt.event.*;
import javax.swing.table.*;
import javax.swing.event.*;

/**
 *
 * @author Bisi
 */
public class Input extends javax.swing.JInternalFrame {

    public Input() {
        super();
        initComponents();
        getValues();
        this.pack();
    }

    private void initComponents() {
        this.setClosable(true);
        this.setMaximizable(true);
        this.setResizable(false);
        this.setIconifiable(true);
        this.setTitle("Main Menu");

        this.setBorder(new LineBorder(Color.black));
        this.setFrameIcon(null);

        this.getContentPane().setLayout(new
        javax.swing.BoxLayout(getContentPane(),
        javax.swing.BoxLayout.Y_AXIS));
        pack();
        this.setVisible(true);
        this.setLocation(100,50);
    }

    private double Aval(int i, int j) {
        double ans;
        if(i==j) {
            ans=1;
        } else {
            ans
            (vol[j]/vol[i])*(1-[i][j]/(1.987*(273.15+T[j]))));
        }
        return ans;
    }

```

```

    }

    //Gamma1 for stage j
    private double gamma1(int j) {
        double ans = Math.exp(1-Math.log(x[1][j] +
x[2][j]*Av[1][2]+x[3][j]*Av[1][3]))-
        x[1][j]/(x[1][j]+x[2][j]*Av[1][2]+x[3][j]*Av[1][3])-
        x[2][j]*Av[2][1]/(x[1][j]*Av[2][1]+x[2][j]+x[3][j]*Av[2]
[3]))-
        x[3][j]*Av[3][1]/(x[1][j]*Av[3][1]+x[2][j]*Av[3][2]+x[3]
[j]));
        return ans;
    }

    //Gamma2 for stage j
    private double gamma2(int j) {
        double ans = Math.exp(-Math.log(x[1][j]*Av[2][1] +
x[2][j] + x[3][j]*Av[2][3] +
        1 - (x[1][j]*Av[1][2]/(x[1][j] +
x[2][j]*Av[1][2] + x[3][j]*Av[1][3]))
        + x[2][j]/(x[1][j]*Av[2][1] + x[2][j] +
x[3][j]*Av[2][3])) +
        x[3][j]*Av[3][2]/(x[1][j]*Av[3][1] +
x[2][j]*Av[3][2] + x[3][j]))));
        return ans;
    }

    //Gamma3 for stage j
    private double gamma3(int j) {
        double ans = Math.exp(1-
Math.log(x[1][j]*Av[3][1]+x[2][j]*Av[3][2]+x[3][j]))-
        x[1][j]/(x[1][j] +
x[2][j]*Av[1][2]+x[3][j]*Av[1][3]))-
        x[2][j]*Av[2][1]/(x[1][j]*Av[2][1]+x[2][j]+x[3][j]*Av[2]
[3]))-
        x[3][j]*Av[3][1]/(x[1][j]*Av[3][1]+x[2][j]*Av[3][2]+x[3]
[j]));
        return ans;
    }

    //Temperature of stage j
    private double T_(int j) {
        double ans = (P - gamma1(j)*satP(1,j)*x[1][j] -
        gamma2(j)*satP(2,j)*x[2][j] -
        gamma3(j)*satP(3,j)*x[3][j])/P;
        return ans;
    }

    //Saturated Pressure by Antoinies Equation
    private double satP(int i, int j) {
        return( Math.exp(A[i]- B[i]/(T[j]+273+C[i])));
    }

    //Relative Volatility value by Raoult's Modified Law
    private double alpha(int i, int j) {
        double ans=0;
        switch(i) {

```

```
        case 1:
            ans = gamma1(j)*satP(1,j)/(
gamma2(j)*satP(2,j) );
            break;
        case 2:
            ans = gamma2(j)*satP(2,j)/(
gamma2(j)*satP(2,j) );
            break;
```

```

K = new double[4][10];

V = 10;
R = 2;
D = V/(R+1);
D=0;
L = V - D;
P = 101.3;

//vapor Pressure Using Antoine Equation
//A[1] = 7.11714; B[1] = 1210.595; C[1] = 229.664;
//A[2] = 6.95465; B[2] = 1170.966; C[2] = 226.232;
//A[3] = 8.08097; B[3] = 1582.271; C[3] = 239.726;
A[1] = 6.038757; B[1] = 1149.261; C[1] = -43.150;
A[2] = 7.025886; B[2] = 1474.078; C[2] = -44.020;
A[3] = 5.936790; B[3] = 1257.840; C[3] = -53.415;

//Binary interaction Parameters for wilson Model
l_[1][2] = 116.1171; l_[1][3] = -114.4047; l_[2][3]
= -506.8519;
l_[2][1] = -506.8519; l_[3][1] = 545.2942; l_[3][2]
= 1694.0241;

vol[1] =74.05; vol[2] =80.67; vol[3] =40.73;

for(int i =1; i <=3; i++) {
    for(int j =1; j <=3; j++) {
        Av[i][j] = Aval(i,j);
    }
}
Av[1][2] = .5004;    Av[2][3]= 0.1072;    Av[1][3]=
0.8862;
Av[2][1] = .4804;    Av[3][2]= .08442;    Av[3][1]=
.9287;

for(int i =1; i <=3; i++) {
    for(int j =0; j <=8; j++) {
        x[i][j] = 0.1;
        M[j] = 0.005;
        T[j] = 57.58;
    }
}
M[0] = 0.01;
//STAGE 9 (Reboiler System)
x[1][9] = 0.3234;
x[2][9] = 0.2236;
x[3][9] = 0.4530;
M[9] = 100;

T[9] = 57.58;

```

```

k3 = new double[4][10];
k4 = new double[4][10];
do {
    for (int i = 1; i <=3; i++){
        k1[i][9] = delta* Stage9(x[i][8], x[i][9], i);
        for(int j = 8; j >=1; j--) {
            k1[i][j] = delta* Stage8_1(x[i][j-1],
x[i][j], i, j);
        }
        k1[i][0] = delta* Stage0(x[i][0], i);
    }
    for (int i = 1; i <=3; i++){
        k2[i][9] = delta* Stage9(x[i][8]+0.5*k1[i][8],
x[i][9]+0.5*k1[i][9], i);
        for(int j = 8; j >=1; j--) {
            k2[i][j] = delta* Stage8_1(x[i][j-1]+0.5*k1[i][j-1], x[i][j]+0.5*k1[i][j], i, j);
        }
        k2[i][0] = delta* Stage0(x[i][0]+0.5*k1[i][0],
i);
    }
    for (int i = 1; i <=3; i++){
        k3[i][9] = delta* Stage9(x[i][8]+0.5*k2[i][8],
x[i][9]+0.5*k2[i][9], i);
        for(int j = 8; j >=1; j--) {
            k3[i][j] = delta* Stage8_1(x[i][j-1]+0.5*k2[i][j-1], x[i][j]+0.5*k2[i][j], i, j);
        }
        k3[i][0] = delta* Stage0(x[i][0]+0.5*k2[i][0],
i);
    }
    for (int i = 1; i <=3; i++){
        k4[i][9] = delta* Stage9(x[i][8]+k3[i][8],
x[i][9]+k3[i][9], i);
        for(int j = 8; j >=1; j--) {
            k4[i][j] = delta* Stage8_1(x[i][j-1]+k3[i][j-1], x[i][j]+k3[i][j], i, j);
        }
        k4[i][0] = delta* Stage0(x[i][0]+k3[i][0], i);
    }
}

time = time + delta;
System.out.println("time: "+time);

for (int i = 1; i <=3; i++){
    x[i][9] = x[i][9] + (1/6)*(k1[i][9] +
2*(k2[i][9]+k3[i][9]) + k4[i][9]);
    y[i][9] = Y(i,9);
    T[9] = T_(9);
    for(int j = 8; j >=1; j--) {
        x[i][j] = x[i][j] + (1/6)*(k1[i][j] +
2*(k2[i][j]+k3[i][j]) + k4[i][j]);
        y[i][j] = Y(i,j);
        T[j] = T_(j);
        System.out.println(k1[i][j] + ";" + "\n" +
k2[i][j] + ";" + "\n" +k3[i][j] + ";" + "\n" +k4[i][j] + ";" );
    }
    x[i][0] = x[i][0] + (1/6)*(k1[i][0] +
2*(k2[i][0]+k3[i][0]) + k4[i][0]);
}

```



```

        y[i][0] = Y(i, 0);
        T[0] = T_(0);
    }
} while(time < 2000 );

    createTable();
}

private void createTable() {
    MyTableModel mine = new MyTableModel();

    table = new JTable(mine);
    table.setPreferredSize(new
Dimension(500, 200) );
    table.setBorder(new EmptyBorder(0,0,0,0));
    JScrollPane scrollPane = new JScrollPane(table);
    scrollPane.setBorder(new EmptyBorder(0,0,0,0));
    table.setToolTipText("Results");
    table.setAutoCreateColumnsFromModel(true);
    table.setName("Simulated");

    getContentPane().add(scrollPane); //,
java.awt.BorderLayout.NORTH
    pack();
}
class MyTableModel extends AbstractTableModel {
    final String[] columnNames = {"Stages",
"T","M","x1", "x2", "x3","y1", "y2", "y3"};

    final Object[][] data = {
        {"Condenser", new Float(T[0]),new
Float(M[0]), new Float(x[1][0]), new Float(x[2][0]), new
Float(x[3][0]), new Float(y[1][0]), new Float(y[2][0]), new
Float(y[3][0])},
        {"Stage 1", new Float(T[1]), new
Float(M[1]), new Float(x[1][1]), new Float(x[2][1]), new
Float(x[3][1]), new Float(y[1][1]), new Float(y[2][1]), new
Float(y[3][1])},
        {"Stage 2" new Float(T[2]) new

```

```

        {"Stage 7", new Float(T[7]), new
Float(M[7]), new Float(x[1][7]), new Float(x[2][7]), new
Float(x[3][7]), new Float(y[1][7]), new Float(y[2][7]), new
Float(y[3][7])},
        {"Stage 8", new Float(T[8]), new
Float(M[8]), new Float(x[1][8]), new Float(x[2][8]), new
Float(x[3][8]), new Float(y[1][8]), new Float(y[2][8]), new
Float(y[3][8])},
        {"Reboiler", new Float(T[9]), new
Float(M[9]), new Float(x[1][9]), new Float(x[2][9]), new
Float(x[3][9]), new Float(y[1][9]), new Float(y[2][9]), new
Float(y[3][9])}
};

```

```

    public int getColumnCount() {
        return columnNames.length;
    }

    public int getRowCount() {
        return data.length;
    }

    public String getColumnName(int col) {
        return columnNames[col];
    }

    public Object getValueAt(int row, int col) {
        return data[row][col];
    }

    public boolean isCellEditable(int row, int col) {
        return true;
    }

    public void setValueAt(Object value, int row, int
col) {
        data[row][col] = value;
        fireTableCellUpdated(row, col);
    }

    public Class getColumnClass(int c) {
        return getValueAt(0, c).getClass();
    }

}

```

```

// Variables declaration - do not modify//GEN-BEGIN:variables

```

```

    private double h;
    private double[][] x, y, K, L, AV, G, PS;
    private double V, L;
    private double D, R, P, Rg;
    private double[] A, B, C, T, M, vol;
    private JTable table;
// End of variables declaration//GEN-END:variables

```

}

.

Corel Uninstaller Wizard

Modelling and Simulation of Batch Distillation

File Edit Help

Main Menu

Stages	T	M	x1	x2	x3	y1	y2	y3
Condenser	0.998	0.01	0.1	0.1	0.1	0.715	0.246	0.039
Stage 1	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 2	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 3	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 4	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 5	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 6	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 7	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Stage 8	0.998	0.005	0.1	0.1	0.1	0.715	0.246	0.039
Reboiler	0.967	1.00	0.323	0.224	0.453	0.298	0.677	0.024

Start | Windows Media Player | Add or Remove Progr... | Corel Uninstaller Wizard | D:\WINDOWS\System... | Modelling and Simul... | Desktop 8:03 PM

**REFERENCES**

1. Bosley, J.R. and Thomas F. Edgar(1994), An efficient dynamic model for batch distillation, *J. Proc. Cont.*.
2. Galindez, H. and A. Fredenslund(1988), "Simulation of Multicomponent Batch Distillation Processes", *Computer Chemical Engineering*.
3. Kooijman, H.A. and R. Taylor(1995), "A Non-Equilibrium Model For Dynamic Simulation of Tray Distillation Columns", *AIChE J.*, **41**, 1852.
4. Sadotomo, H. and K. Miyahara(1983), "Calculation procedure for multicomponent batch distillation", *International Chem. Engineering*.
5. Skogestad, S., B. Wittgens, E. Sørensen, and R. Littø(1997), "Multivessel Batch Distillation", *AIChE J.*, **43**, 971.
6. McCabe, Warren. *Unit Operations of Chemical Engineering*, Fifth Edition. McGraw-Hill Inc, 1993, Chapters 18 and 19.
7. *Distillation Column Design*. Copyright 1997.  
<http://lorien.ncl.ac.uk/ming/distil/distil0.htm>
8. Betlem, B.H.L., Krijnsen, H.C. and Huijnen, H (1998). Optimal batch distillation control based on specific measures, *Chemical Engineering Journal* 71, p111-126
9. R K Sinnott (1999), *Coulson & Richardson's Chemical Engineering*, Third Edition, Butterworth-Heinemann, Volume 6 Chapter 8.
10. King, C. Judson, *Separation Processes*, Second Edition. McGraw-Hill, Inc., 1980, Chapters 4-6.