

# bradscholars

**Optimal design and operation of multivessel batch distillation with fixed product demand. Modelling, simulation and optimisation of design and operation parameters in multivessel batch distillation under fixed product demand scenario and strict product specifications using simple dynamic model in gPROMS.**

Item Type	Thesis
Authors	Mahmud, Mohamed Taher Mustafa
Rights	<a href="http://creativecommons.org/licenses/by-nc-nd/3.0/">&lt;a rel="license" href="http://creativecommons.org/licenses/by-nc-nd/3.0/"&gt;&lt;img alt="Creative Commons License" style="border-width:0" src="http://i.creativecommons.org/l/by-nc-nd/3.0/88x31.png" /&gt;&lt;/a&gt;&lt;br /&gt;The University of Bradford theses are licenced under a &lt;a rel="license" href="http://creativecommons.org/licenses/by-nc-nd/3.0/"&gt;Creative Commons Licence&lt;/a&gt;.</a>
Download date	2026-06-08 02:05:28
Link to Item	<a href="http://hdl.handle.net/10454/4435">http://hdl.handle.net/10454/4435</a>



## **University of Bradford eThesis**

This thesis is hosted in [Bradford Scholars](#) – The University of Bradford Open Access repository. Visit the repository for full metadata or to contact the repository team



© University of Bradford. This work is licenced for reuse under a [Creative Commons Licence](#).

**OPTIMAL DESIGN AND OPERATION OF MULTIVESSEL  
BATCH DISTILLATION WITH FIXED  
PRODUCT DEMAND**

Modelling, simulation and optimisation of design and operation parameters in  
multivessel batch distillation under fixed product demand scenario  
and strict product specifications using simple dynamic model in gPROMS

**Mohamed Taher Mustafa MAHMUD**

*BSc Chem. Eng.*

**Submitted for the Degree of Master of Philosophy**

**School of Engineering, Design and Technology**

**University of Bradford**

**UK**

**2010**

# OPTIMAL DESIGN AND OPERATION OF MULTIVESSEL BATCH DISTILLATION WITH FIXED PRODUCT DEMAND

**Keywords:** Conventional batch distillation, Multivessel batch distillation, Design, Operation, Product sequence, Profitability, Modelling, Optimisation

## ABSTRACT

Increased interest in unconventional batch distillation column configurations offers new opportunities for increasing the flexibility and energy efficiency of batch distillation. One configuration of particular interest is multivessel batch distillation column, which can be viewed as a generalization of all previously studied batch column configuration.

In this work, for the first time the optimal design and operation tasks are developed for multivessel batch distillation with strict product specifications under fixed product demand.

Also, in this work, two different operation schemes defined as *STN* (State Task Network) in terms of the option and numbers of off-cuts were considered for binary and ternary separation. Both the vapour load and number of stages in each column section together with the production sequence are optimised to achieve maximum profit function.

The performance of the multivessel batch distillation column is evaluated against the performance of conventional batch column with a simple dynamic model using binary and ternary mixtures. It has been found that profitability improves with the multivessel system in both separations.

gPROMS, a user-friendly, software is used for the modeling, simulation, and optimisation.

# DEDICATED

*This thesis is dedicated to:*

*My late father and mother, may Allah have mercy on their souls, whom both passed away before seeing the completion of this work.*

*I am also highly indebted to my wife who, through her patience and tolerance, took the best care of our children and me, and for her invaluable encouragement and unlimited support throughout my work.*

*Also to my children, who represent the new generation and for whom I am willing to take the responsibility in providing them with a good and happy future.*

## ACKNOWLEDGMENT

I would like to express my sincere gratitude to my supervisor Professor I. M. Mujtaba for his invaluable guidance and advice, continuous co-operation, valuable comments, suggestions, unlimited help and support throughout this work.

I wish to express my sincere thanks to my wife for the time and effort that she invested for my sake and for sake of our children and her boundless patience for the whole period during my study.

Also very special thanks to my father in-law Salah El-Din for his unlimited support and co-operation and his assistance. I also would like to offer my thanks to all friends that I have known in Bradford University for supporting me.

I would like to acknowledge all those at the Libyan Petroleum Institute (LPI) who have supported my research, and given me their trust to get this degree.

Last, but not least, I want to thank my brothers and sisters for their love, support, encouragement, and blessing to undertake my postgraduate study.

# LIST OF CONTENTS

<i>Contents</i>	<i>Page</i>
<b>Abstract</b>	<i>ii</i>
<b>Dedications</b>	<i>iii</i>
<b>Acknowledgement</b>	<i>iv</i>
<b>List of Contents</b>	<i>v</i>
<b>List of Tables</b>	<i>x</i>
<b>List of Figures</b>	<i>xii</i>
<b>Nomenclature</b>	<i>xiv</i>
<b>Chapter 1: Introduction</b>	
1.1. Batch Processes	1
1.2. Batch Distillation	2
1.3. Types of Batch Distillation	3
1.4. Multivessel Batch Distillation	7
1.5. Scope of the research	10
1.6. Aims and Objectives of the Thesis	12
1.7. Outline of the Thesis	13
<b>Chapter 2: Literature Review</b>	
2.1. Introduction	16
2.2. Continuous Distillation Column	16

2.3.	Batch Distillation Column	18
2.4.	Conventional Batch Distillation (CBD)	20
2.5.	Non Conventional Batch Distillation Methods	23
2.5.1.	Inverted Batch Distillation Column (IBD)	23
2.5.2.	Middle Vessel Batch Distillation Column (MVBD)	25
2.5.3.	Multivessel Batch Distillation Column (MultiVBD)	26
2.6.	Total reflux operation Policies for (MultiVBD) Column	31
2.7.	Conclusions	33

### **Chapter 3: Review of Past Work**

3.1.	Introduction	35
3.2.	Process Modelling	35
3.3.	Process Simulation	37
3.4.	Process Optimisation	39
3.5.	Modelling and Simulation of Multivessel Batch Distillation	41
3.6.	Optimisation Studies of Multivessel Batch Distillation	41
3.7.	Process Simulator	44
3.7.1.	gPROMS Simulator	45
3.7.2.	Feature of gPROMS	45
3.8.	Defining a Task/Process/Optimisation	47
3.9.	Conclusions	51

### **Chapter 4: Process Models**

4.1.	Introduction	52
4.2.	Simple Model	52

4.3.	Simple Model for Conventional Batch Distillation	53
4.4.	Simple Model for Multivessel Batch Distillation	56
4.5.	Conclusion	59

## **Chapter 5: Optimal Design and Operation of Binary Distillation**

5.1	Introduction	60
5.2.	Operation Sequence	61
5.3.	Optimisation Problem with Fixed Product Demand	65
5.4.	Example Problems	68
5.4.1.	Effect of Number of Stages	71
5.4.1.1	Results	72
5.4.2.	Effect of Vapour Load	73
5.4.2.1	Results	73
5.4.3.	Simultaneous Optimisation of Number of Stages and Vapour Load	74
5.4.3.1	Results	75
5.5.	Conclusions	78

## **Chapter 6: Multicomponent Multivessel Batch Distillation Column– STN 1**

6.1.	Introduction	79
6.2.	Case Study and Comparison of Multivessel with Conventional Columns	82
6.2.1.	Product Demand and Specifications	82
6.2.2.	Objective Function and Optimisation Problem Formulation	84
6.2.3.	Results and Discussions	85
6.3.	Conclusions	90

## **Chapter 7: Multicomponent Multivessel Batch Distillation Using Other STNs**

7.1.	Introduction	92
7.2.	Optimal Operation and Design with STN-2: ( <i>Case Study-1.1</i> )	93
7.2.1.	Sample Calculations	96
7.2.2.	Profit Calculations	99
7.3.	Optimal Operation and Design with STN-2: ( <i>Case Study-1.2</i> )	101
7.3.1.	Profit Calculations	104
7.4.	Optimal Operation and Design with STN-2: ( <i>Case Study-1.3</i> )	106
7.4.1.	Profit Calculations	109
7.5.	Conclusions	111
7.6.	Optimal Operation and Design with STN-3: ( <i>Case Study-2.1</i> )	112
7.6.1.	Sample Calculations	116
7.6.2.	Profit Calculations	117
7.7.	Optimal Operation and Design with STN-3: ( <i>Case Study-2.2</i> )	120
7.7.1.	Profit Calculations	121
7.8.	Optimal Operation and Design with STN-3: ( <i>Case Study-2.3</i> )	124
7.8.1.	Profit Calculations	125
7.9.	Conclusions	128

## **Chapter 8: Conclusion and Future Recommendations**

8.1.	Conclusions	130
8.1.1.	Process Modelling and Optimisation	130
8.1.2.	Operation and Design Optimisation	131
8.1.3.	Operation and Design Optimisation for Ternary Distillation	132
8.1.4.	Operation and Design Optimisation of <i>MultiVBD</i> Distillation	132

8.2. Future Recommendations	133
<b>Reference</b>	135
<b>Appendix</b>	147

# LIST OF TABLES

<i>Contents</i>	<i>Page</i>
3.1. Summary of the Past Work on Optimisation of MultiVBD Column	43
5.1. Input Data for Binary Distillation of CBD and MultiVBD Column	70
5.2. Summary of the Results – Effect of $N$ with Fixed $V$	72
5.3. Summary of the Results – Effect of $V$ with Fixed $N$	73
5.4. Maximum Profit – (Optimum $V$ and $N$ )	75
5.5. Summary of the optimisation for different processes (Maximum Profit)	77
6.1. Input Data for Ternary Distillation of CBD and MultiVBD	83
6.2. Profit Profile for CBD and MultiVBD Columns with Desired $N_B$	86
6.3. Summary of the Result Using (Profit Function - 1)	86
6.4. Maximum Profit Using (Profit Function - 2)	88
6.5. Product Specifications of Multivessel Batch Distillation Column	88
7.1. Possible Product Profiles for STN-2 ( <i>Case-1.1</i> ) Based on Mass Balance	98
7.2. Optimal Operation and Design for STN-2 ( <i>Case-1.1</i> )	100
7.3. Possible Product Profiles for STN-2 ( <i>Case-1.2</i> ) Based on Mass Balance	103
7.4. Optimal Operation and Design for STN-2 ( <i>Case-1.2</i> )	105
7.5. Possible Product Profiles for STN-2 ( <i>Case-1.3</i> ) Based on Mass Balance	108
7.6. Optimal Operation and Design for STN-2 ( <i>Case-1.3</i> )	110
7.7. Possible Product Profiles for STN-3 ( <i>Case-2.1</i> ) Based on Mass Balance	117
7.8. Optimal Operation and Design for STN-3 ( <i>Case-2.1</i> )	119

7.9.	Possible Product Profiles for STN-3 ( <i>Case-2.2</i> ) Based on Mass Balance	121
7.10.	Optimal Operation and Design for STN-3 ( <i>Case-2.2</i> )	123
7.11.	Possible Product Profiles for STN-3 ( <i>Case-2.3</i> ) Based on Mass Balance	125
7.12.	Optimal Operation and Design for STN-3 ( <i>Case-2.3</i> )	127

# LIST OF FIGURES

<i>Figure</i>	<i>page</i>
1.1. Conventional Batch Distillation Column	4
1.2. Inverted Batch Distillation Column (IBD)	5
1.3. Middle Vessel Batch Distillation Column (MVBD)	6
1.4. Continuous Distillation Column	7
1.5. Multivessel Batch Distillation Column (MultiVBD)	8
2.1. Continuous Distillation Column	17
2.2. Crude Oil Distillation Column	18
2.3. Conventional Batch Distillation Column (CBD)	21
2.4. Typical Instant Distillate Composition Profile	22
2.5. Inverted Batch Distillation Column (IBD)	24
2.6. Middle Vessel Batch Distillation Column (MVBD)	25
2.7. Multivessel Batch Distillation Column (MultiVBD)	27
3.1. An Overview of the <i>gPROMS</i> (Part of the Models File)	48
3.2. An Overview of the <i>gPROMS</i> (Part of the Processes File)	49
3.3. An Overview of the <i>gPROMS</i> (Part of the Optimizations File)	50
4.1. Conventional Batch Distillation Column (CBD)	54
4.2. Connection of Plates and Vessel for (MultiVBD)	57
5.1. Conventional Batch Column (CBD)	62
5.2. Multivessel Batch Distillation with Two Column Sections	63

5.3.	STN for Binary Batch Column	64
5.4.	Composition of Main Cut and Off-Cut for <i>MultiVBD</i> column ( <i>Case - 3</i> )	76
6.1.	STN for Multivessel and Conventional Columns with Two Main-Cuts	81
6.2.	Composition of Main-Cut 1 of <i>MultiVBD</i> Column	88
6.3.	Composition of Off-Cut 1 of <i>MultiVBD</i> Column	89
6.4.	Composition of Main-Cut 2 of <i>MultiVBD</i> Column	89
6.5.	Composition of Bottom Residue of <i>MultiVBD</i> Column	90
7.1.	STN-2 with Each Off-Cut Followed by Main-Cuts	93
7.2.	STN-3 with Two Main-Cuts and One Off-Cut in Between	112
7.3.	Multivessel Batch Distillation with Two Column Sections	113

# NOMENCLATURE

$\alpha$	relative volatility
$A$	constant for operating cost equation.(8000).
$ACC$	annualised capital cost (\$/year).
$B_o$	total initial charge (kmol/batch).
$B_1$	first total bottom product (kmol/batch).
$B_2$	intermediate and/or bottom product (kmol/batch).
$B_3$	intermediate and/or bottom product (kmol/batch).
$B_f$	bottom residue or final product (kmol/batch).
$C_1$	top product price, for profit equation (\$/kmol).
$C_2$	second product price, for profit equation (\$/kmol).
$C_3$	raw material cost, for profit equation (\$/kmol).
$C_{Bo}$	cost of fresh feed mixture (\$/kmol).
$CBD$	conventional batch distillation.
$C_{fc}$	fixed operating cost (5.0 \$/h).
$D$	total distillate product (kmol)
$D_1$	main cut-1 (kmol).
$D_2$	main cut-2 (kmol)
$D_3$	main cut-3 (kmol)
$DAEs$	differential and algebraic equations.
$F_i$	liquid stream leaving vessel -1 (mole/hr).
$H$	operating time per year (h/year)

$H_f$	vessel-1 holdup or feed tank-1 (kmol).
$H_n$	reboiler holdup (kmol).
$H_c$	condenser holdup (kmol).
$i$	component $i$
$IBD$	inverted batch distillation.
$j$	tray $j$ .
$k$	vapour-Liquid equilibrium constant.
$K_1$	constant for Annualised capital costs equation (1500).
$K_2$	constant for Annualised capital costs equation (9500).
$K_3$	utility costs coefficient (constant for operating cost equation 180)
$L$	liquid flow rate (kmol /hr).
$L_{fi}$	liquid rate feed holdup on plate $nt$ (kmol /hr)
$M_c$	molar holdup of $c$ condenser (kmol /hr)
$M_j$	molar holdup of $j$ tray (kmol /hr)
$M_n$	molar holdup of $n$ reboiler (kmol /hr)
$MPSSS$	multi-pass sequential steady state.
$MVBD$	middle vessel batch distillation.
$MultiVBD$	multivessel batch distillation.
$N$	total Number of trays
$N_B$	number of batches (batch/ year).
$N_c$	number of components.
$nb$	trays number of bottom section.
$nm$	trays number of middle section.
$nt$	trays number of top section

$OC$	operating cost (\$/year).
$OC_b$	operating cost/batch (\$/batch).
$ODEs$	ordinary differential equations.
$P$	profit (\$/year).
$Q_c$	condenser duty.
$Q_h$	reboiler heat duty.
$R_1$	off-cut 1 (kmol).
$R_2$	off-cut 2 (kmol).
$r$	reflux ratio
$SPSS$	single pass steady state.
$SPSSS$	single pass sequential steady state.
$STN$	state task network.
$t_b$	batch time (hr).
$t_s$	set up time (constant = 0.5 hr).
$V$	vapour load (kmol/hr).
$V_B$	vapour stream leaving the reboiler (mole/hr).
$V_j$	stream leaving plate $j$ (mole/hr).
$x$	liquid composition (mole fraction).
$x^1_{Bo}$	compositions of initial charge of component 1.
$x^2_{Bo}$	compositions of initial charge of component 2.
$x^3_{Bo}$	compositions of initial charge of component 3.
$x_f$	feed composition (mole fraction).
$x_j$	liquid composition of the component $i$ on plate $j$ (mole fraction).

$x_{D1}^1$	specified molefractions of main-cut-1 of component 1.
$x_{D2}^1$	specified molefractions of main-cut-2 of component 2.
$x_{D3}^1$	specified molefractions of main-cut-3 of component 3.
$x_{R1}^1$	molefractions 1 of off-cut of component $l$ .
$x_{R1}^2$	molefractions 2 of off-cut of component $l$ .
$x_{R1}^3$	molefractions 3 of off-cut of component $l$ .
$y_j$	vapour composition at tray $j$ .

# CHAPTER 1

## INTRODUCTION

### 1.1 Batch Processes

In the 1950s, chemical engineers might have to transform old fashioned batch processes into modern continuous ones (Rippin, 1983). Today, a significant proportion of the world's chemical by volume and a much larger proportion by value is still made in batch plants.

Parakrama (1985) reported that 99 batch processes were in operation in 74 UK manufacturing companies. Among these, 80% plants were producing chemical in growing markets. Moreover, many more products, in fact made in batch plants on economic grounds (Rippin, 1991).

Batch productions are usually carried out in standardised types of many equipment, which can be easily adapted and if necessary reconfigured to produce many other different products. It is especially suitable for low volume of material to be separated, high value products such as fine fragrances, chemical, polymers, pharmaceuticals, and biochemical or other fine chemicals. These products could be manufactured in few days or few batches. It is usually economically more efficient to manufacture them in a facility such as multipurpose batch plant (the batch plant could be used for separation of chemical and in the next batch for crude oil and once for separation of perfumes, etc.).

## 1.2 Batch Distillation

The application of distillation ranges from enhancing the alcohol content of beverages to the prime separation technique in the chemical industry. This range accelerated once distillation was recognised as an effective means of separating crude oil into various products. Distillation is a process of physically separating a mixture into two or more products that have different boiling points, when a liquid mixture of two volatile materials is heated, the vapour that comes off will have a higher concentration of the more volatile (*i.e.*, lower boiling-point) material than the liquid from which it was evolved.

Batch distillation is one of the major operations used in the chemical and pharmaceutical industry for the separation of liquid mixtures into their components. The distillation can be performed as either a continuous or a batch process. In a single batch distillation column, multicomponent mixtures can be separated into a number of product fractions, whereas in continuous distillation a sequence of columns is necessary to perform the same task. For a multicomponent liquid mixture with ( $N_c$ ) number of components, usually ( $N_c - 1$ ) number of continuous columns will be necessary to separate all the components from the mixture.

Batch distillation has the advantage in many cases and it is used in industries where high purity products are produced and used for purifying of products or recovering solvents or valuable reactants from waste streams. Batch distillation has another advantage of being much more flexible than continuous distillation. Also completely different mixtures (which have different boiling point) can be separated using batch distillation. This is a big advantage with today's frequently changing product specification requirements and market demand. Furthermore batch distillation often means simpler operation and lower capital

cost than continuous distillation (Skogestad *et al.*, 1997). The fact that the use of batch distillation as well as the competitiveness in chemical industry has increased in recent years (Low and Sorensen, 2005).

A single mixture (binary or multicomponent) can be separated into several products (*single separation duty*) and multiple mixtures (binary or multicomponent) can be processed, each producing a number of products (*multiple separation duties*) using only one Conventional batch distillation *CBD* (Logsdon *et al.*, 1990; Mujtaba and Macchietto, 1996; Sharif *et al.*, 1998).

Finally, in pharmaceutical and food industries, the product specification or product tracking is very important in the face of strict quality control and batch wise production provides the batch identity (Low and Sorensen, 2003).

### **1.3 Types of Batch Distillation**

There are two major types of batch distillation columns, each one designed to perform specific types of separation, and there are; Conventional and Unconventional batch distillation (Mujtaba, 2004). Alternative configurations, collectively identified as unconventional distillation column have been found in certain cases to be more advantageous. More details are considered and discussed in later chapter for conventional and unconventional distillation columns;

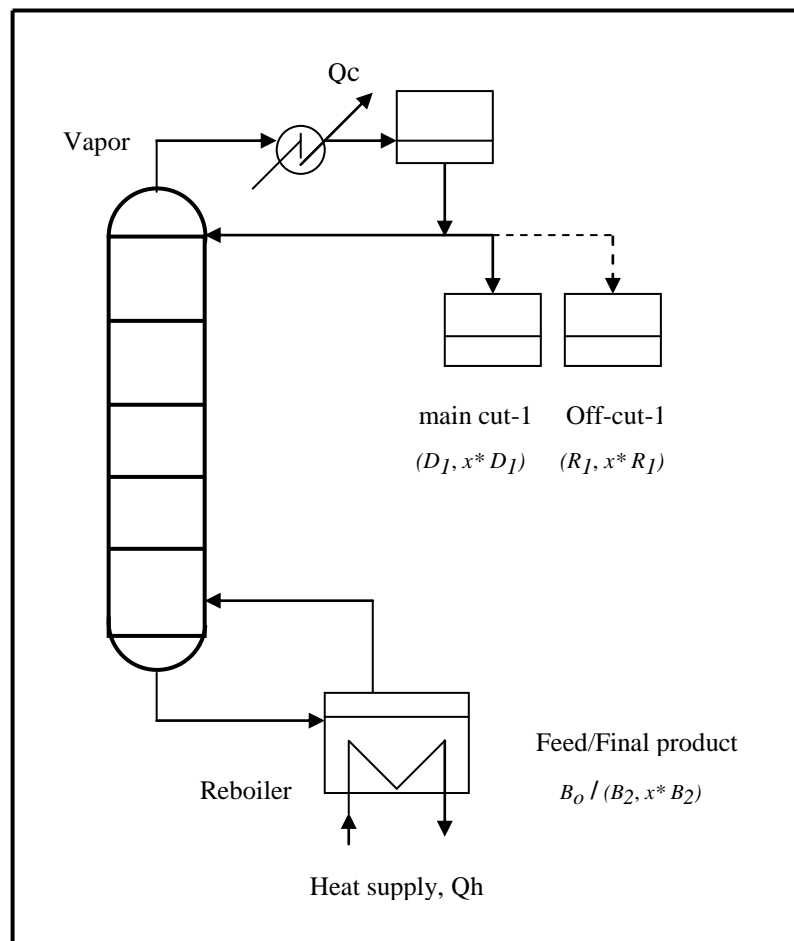
- Conventional Batch Distillation Column (*CBD*) *Figure 1.1.*

The unconventional distillation columns are:

- Inverted Batch Distillation Column (*IBD*) *Figure 1.2*.
- Middle Vessel Batch Distillation Column (*MVBD*) *Figure 1.3*.
- Continuous Column for Batch Distillation or *Single Pass Sequential Steady State* operation. (*SPSSS*) *Figure 1.4*.
- Multivessel Batch Distillation Column (*MultiVBD*) *Figure 1.5*.

◇ **Conventional Batch Distillation Column (CBD)**

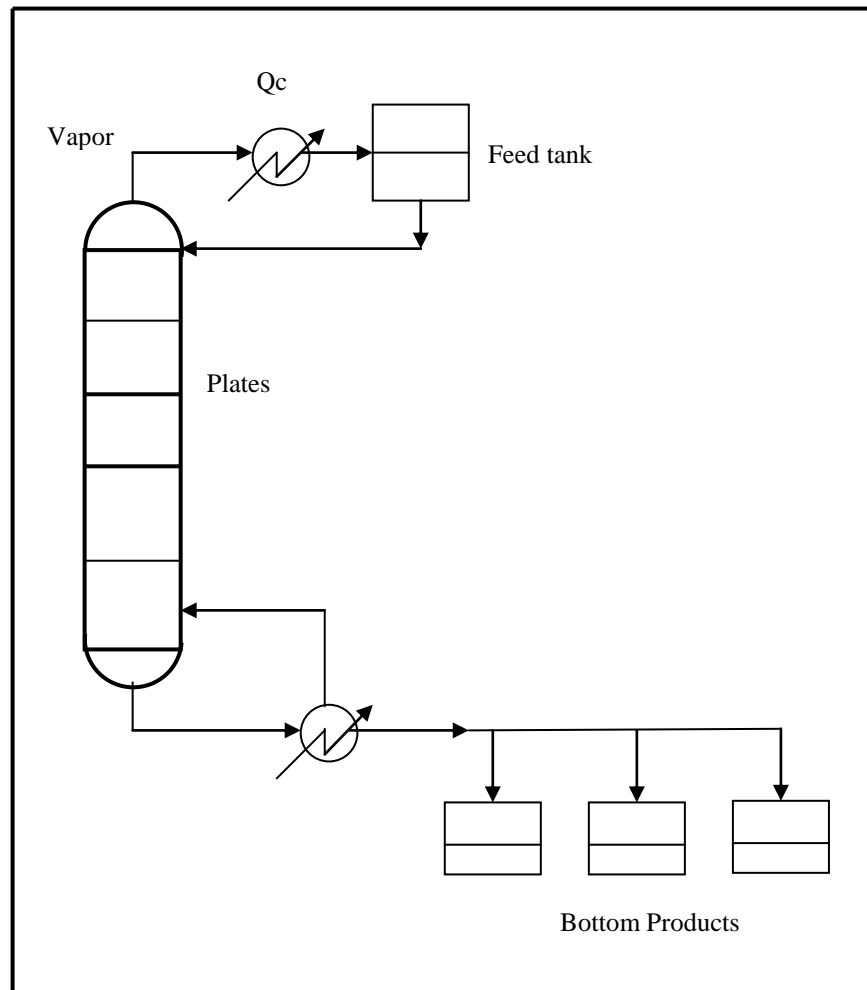
Traditionally, the most popular kind of batch column is conventional (Regular) batch distillation column (CBD) as shown in *Figure 1.1*. This type was presented and discussed in chapter two.



**Figure 1.1:** Conventional Batch Distillation Column (CBD)

◇ **Inverted Batch Distillation Column (IBD)**

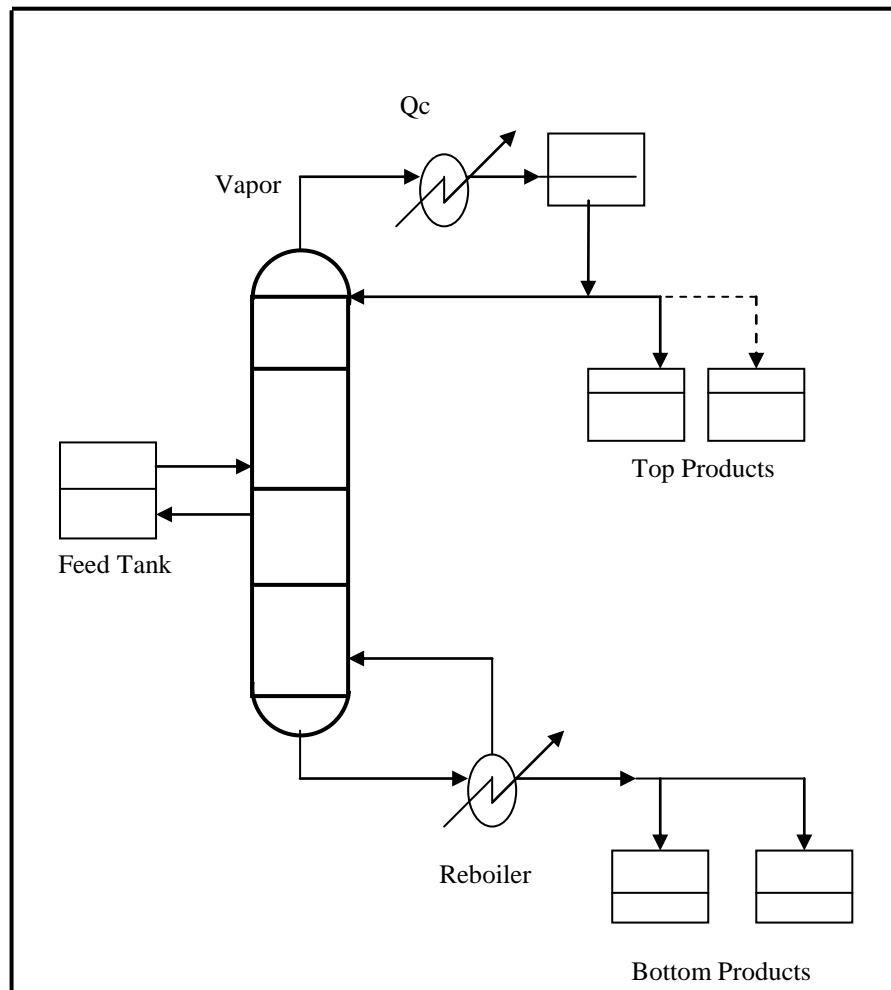
This type of unconventional batch distillation column was presented and discussed in chapter two.



**Figure 1.2:** Inverted Batch Distillation Column (IBD)

◇ **Middle Vessel Batch Distillation Column (MVBD)**

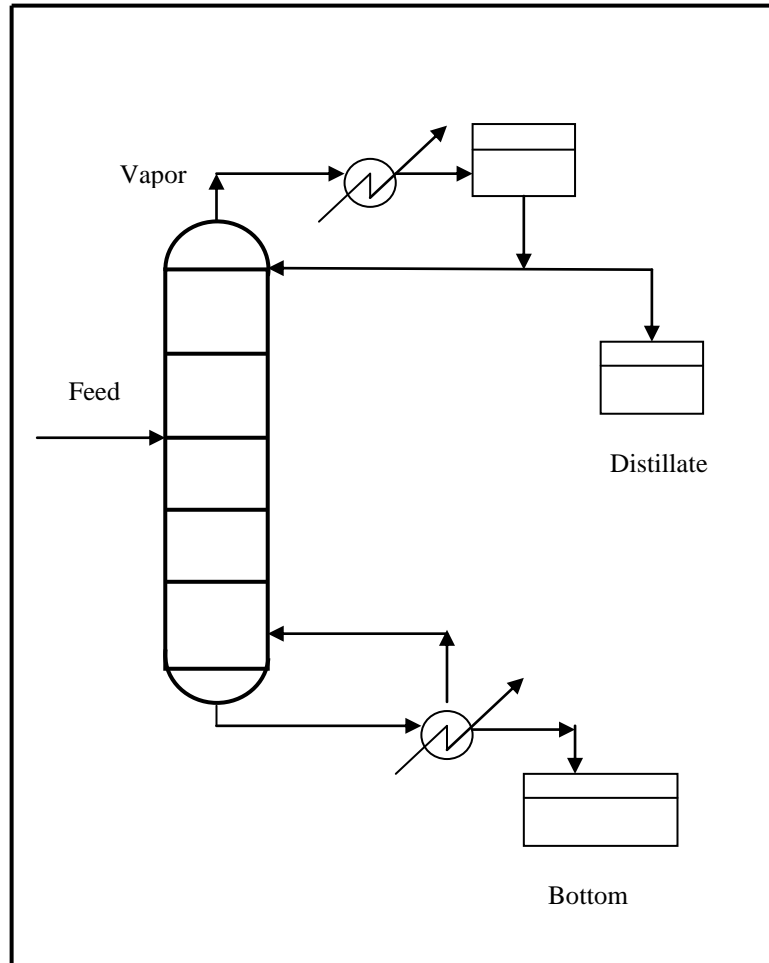
This type of unconventional batch distillation column was presented and discussed in chapter two.



**Figure 1.3:** Middle Vessel Batch Distillation Column (MVBD)

### ◇ Continuous Column for Batch Distillation

This type of unconventional batch distillation column was presented and discussed in chapter two.

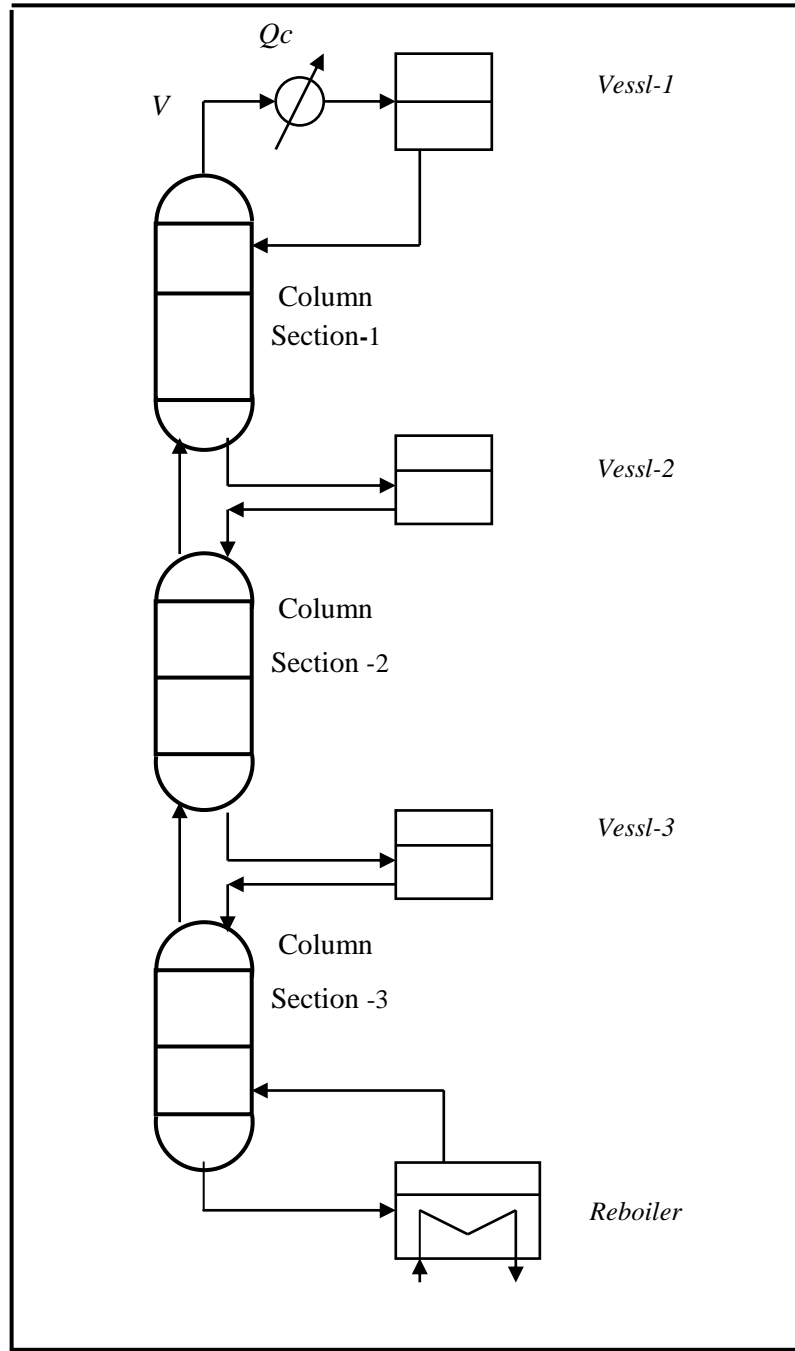


**Figure 1.4:** Continuous Column for Batch Distillation

### 1.4 Multivessel Batch Distillation

The Multivessel batch distillation *MultiVBD* as shown in *Figure 1.5* consists of a condenser drum, several column sections, intermediate vessels and a reboiler, it is useful for the separation of multicomponent mixtures frequently found in the chemical process

industries and it is usually low energy consumption or equivalently for a given heat input, the batch time required to produce the product may be significantly shorter (Furlonge *et al.*, 1999) and the simple operation of the *MultiVBD* is under total reflux, where the feed is distributed among the reboiler, vessels and condenser. All these holdups are kept constant throughout the operation which takes place under total reflux.



**Figure 1.5:** Multivessel Batch Distillation Column (*MultiVBD*)

Furlonge *et al.*, (1999) considered the optimal operation problem for a fixed number of stages and various operating policies such as fixed vessel holdup, variable vessel holdup, and studied the optimum distribution of feed among the reboiler, vessels and reflux drum.

Low and Sorenson (2003) presented the optimal design and operation of *MultiVBD* column. A profit function based on revenue, capital cost and operating cost was maximized while optimising the number of stages in different column sections, reflux ratio, etc. They compared the performance of *MultiVBD* with that of conventional batch distillation column for a number of different mixtures and claimed that *MultiVBD* operation is more profitable. However, for all cases considered in their work, the product specifications and the amount of products were not matched exactly for both configurations and therefore the conclusion is somewhat misleading. Also, reduced batch time will increase the number of batches, this leading to additional production of products in *MultiVBD* column compared to that produced by the conventional column. The optimisation of their study was not geared for fixed product demand and strict product specifications scenarios. That leads to unlimited production of products and their profitability calculations were based on the assumption that all products produced are saleable.

Low and Sorenson (2005) presented the optimal configuration, design and operation of batch distillation column based on overall profitability for a given separation duty. Using rigorous model, the mixed integer dynamic optimisation problem was solved using genetic algorithm. The optimisation of their study was based on a rigorous column model and a comprehensive economics performance index that takes into account production revenue, capital and operating costs was utilised as the base of the configuration design. They found

that the optimal performance was *MultiVBD* configuration over the regular (*CBD*) and inverted configurations.

## 1.5 Scope of the Research

This research is focused on the optimal design and operation parameters for binary and ternary separations of batch distillation with strict product specifications and fixed product demand, which is different than that used in the past under unlimited product demand and with off-cut production. The main issues in batch distillation are:

- Improving the yield in a given batch time or productivity.
- Maximising the profitability for a given product demand and product purity in a given column.
- Minimising the utility cost (operating cost) and annulised capital cost.
- Optimising the design and operation of the systems of Multivessel and Conventional batch distillation columns for a given product demand.

There are specified works that used the *MultiVBD*, for simulation, control and optimisation studies, for example, Hasebe *et al.* (1995), Wittgens *et al.* (1996), Furlonge *et al.* (1999), Low and Sorensen (2003, 2004, and 2005) and Ruiz and Luiz, (2006). There are also works available that compare the optimal operation of the *MultiVBD* system to that of the traditional regular column system *CBD* (Low and Sorensen *et al.*, 2003; 2004 and 2005) The performance indexes used for the comparison included maximum production rate, maximum profit and minimum mean energy consumption.

All studies in the past were assumed that there is an unlimited market demand for amount of products being produced (Low and Sorensen *et al.*, 2003; 2004 and 2005) and without off-cut products to improve the purity or specification requirements.

Off-cut production played an important role in efficient separation of binary and multicomponent mixtures using batch distillation. However the research in this area is handful and all the investigations were concerned with only operation in terms of minimisation of batch time or maximise of productivity (amount of main products per unit time) and no off-cut productions. No considerations were given to market demand of the products; therefore these operation policies would result in under and over production of the products leading to potential revenue losses.

In this work for the first time with off-cut production, both designs (number of stages, vapour load) are optimised which would minimise the capital cost and annualised capital cost while maximising an economic objective function usually the profit ( $P$ ) The effect of off-cut production on the design, operation and profitability in *MultiVBD* column are evaluated against *CBD* column.

For binary mixtures there is usually one main-cut and one off-cut (*Figure 1.1*). The operation of binary system involves carrying out the fractionation until a desired amount has been distilled off. The overhead composition varies during the operation of the cut is desired products (main-cut) while other is intermediate fractions (off-cut) that can be recycled to subsequent batches to obtain further separation. A residual bottom fraction may or may not be recovered as product (Mujtaba, 1989).

For multicomponent mixtures there is usually number of cuts (main-cuts and off-cuts) there is only one sequence of operation (with or without the production of off-specification materials) to separate all the components in a mixture. The only requirements here are to divert the distillate products to different product tanks at specified times.

## 1.6 Aims and Objectives of The Thesis

The aim of this thesis is to study the optimisation of conventional (*CBD*) and unconventional (*MultiVBD*) batch distillation processes involving Binary and Ternary separation systems. Different optimisation problems are formulated and solved.

This research can be highlighted as follows:

1. Develop simple dynamic model for simulation of *Multivessel* and *Conventional* batch distillation columns using different multicomponent system with *gPROMS* software modelling.
2. Develop an optimal design and operation of *MultiVBD* column with off-cut production for Binary and Ternary separation with due regards to the fixed product demand and strict product specifications,
3. Study different scenarios of main cuts and off-cuts (separation tasks) on optimal design and operation of *MultiVBD* column to improve the objective function in terms of (Profit).

The objective of this research is to achieve the following:

- To carry out literature survey on the modelling, simulation and optimisation of batch distillation (Conventional *CBD* and unconventional-*MultiVBD*) column.

- To maximise the overall profit.
- To compare between the performance of *MultiVBD* column and the performance of those obtained (in published literature) using *CBD* on respect to the net profit

In this work, the simulations of the Multivessel batch distillation column under total reflux are presented. The total reflux operation with constant vessel holdup is carried out until the composition of the products in all vessels (reflux drum, intermediate vessels, and reboiler vessel) satisfies the requirements of product, where the holdup of each vessel is calculated in advance by taking into account the amount of feed, feed composition and product specifications.

## **1.7 Outline of the Thesis**

This thesis is organised as follows:

### *Chapter 1: Introduction*

This chapter provides an introduction to the batch processes and batch distillation. Brief descriptions are given for different types of batch distillation column. A review of the Multivessel batch distillation is carried out and outstanding issues are highlighted.

## *Chapter 2: Literature Review*

In this chapter, a general literature reviews on Multivessel batch distillation are considered and discussed. Descriptions for unconventional batch distillation also discussed.

## *Chapter 3: Process Modelling and Optimisation*

This chapter is focused on studies of modelling and simulation of batch distillation including the mathematical optimisations problems. A summary of the past work on optimisation of *MultiVBD* column is also presented. Finally, gPROMS software package is also briefly described.

## *Chapter 4: Process Models*

In chapter four, the simple dynamic models of Multivessel and Conventional batch distillation columns are presented with relevant assumptions made.

## *Chapter 5: Optimal Design and Operation of Binary Batch Distillation under Fixed Product Demand.*

In this chapter, Multivessel and Conventional batch distillation columns are considered with strict product specifications under fixed product demand in terms of maximum profit. The effects of vapour load and number of trays on the optimum design and operation are studied and discussed.

*Chapter 6: Multicomponent Multivessel Batch Distillation Column – STN 1.*

Chapter six presents the optimal operation and design of ternary mixture for the *MultiVBD* Column. The results are evaluated against *CBD* column in respect to the net profit.

*Chapter 7: Multicomponent Multivessel Batch Distillation Column Using Other STNs*

In this chapter, the effect of separation tasks (product sequence) of ternary mixture on the design, operation and overall profitability with two different operation schemes defined as *STN* in terms of number of main-cuts and off-cuts are studied.

*Chapter 8: Conclusion and Future Recommendation*

This chapter gives final conclusions and recommendations of the above studies.

# CHAPTER 2

## LITERATURE REVIEW

### 2.1 Introduction

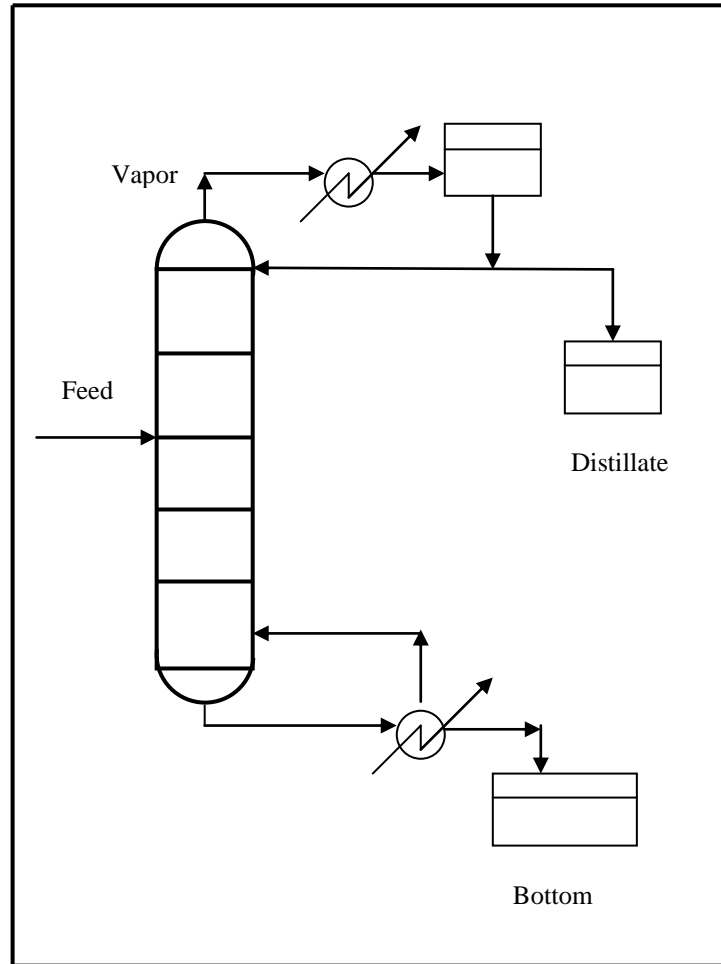
Batch distillation is an important unit operation used in many chemical industries, and in particular in the manufacture of fine chemicals and specialised products such as essential oils, perfume, pharmaceutical and petroleum products.

In this chapter, the background of continuous distillation column, conventional and unconventional batch distillation are presented and discussed. Multivessel batch distillation falls under the category of unconventional batch distillation. While the conventional batch distillation *CBD* column had received much more attention, the researches in Multivessel batch distillation *MultiVBD* column had received less attention (handful). The analysis of the *MultiVBD* column has tended to focus exclusively on the operation of the system, that is, the different operating policies and their on-line control schemes implementation, which are also discussed in this chapter.

### 2.2 Continuous Distillation Column

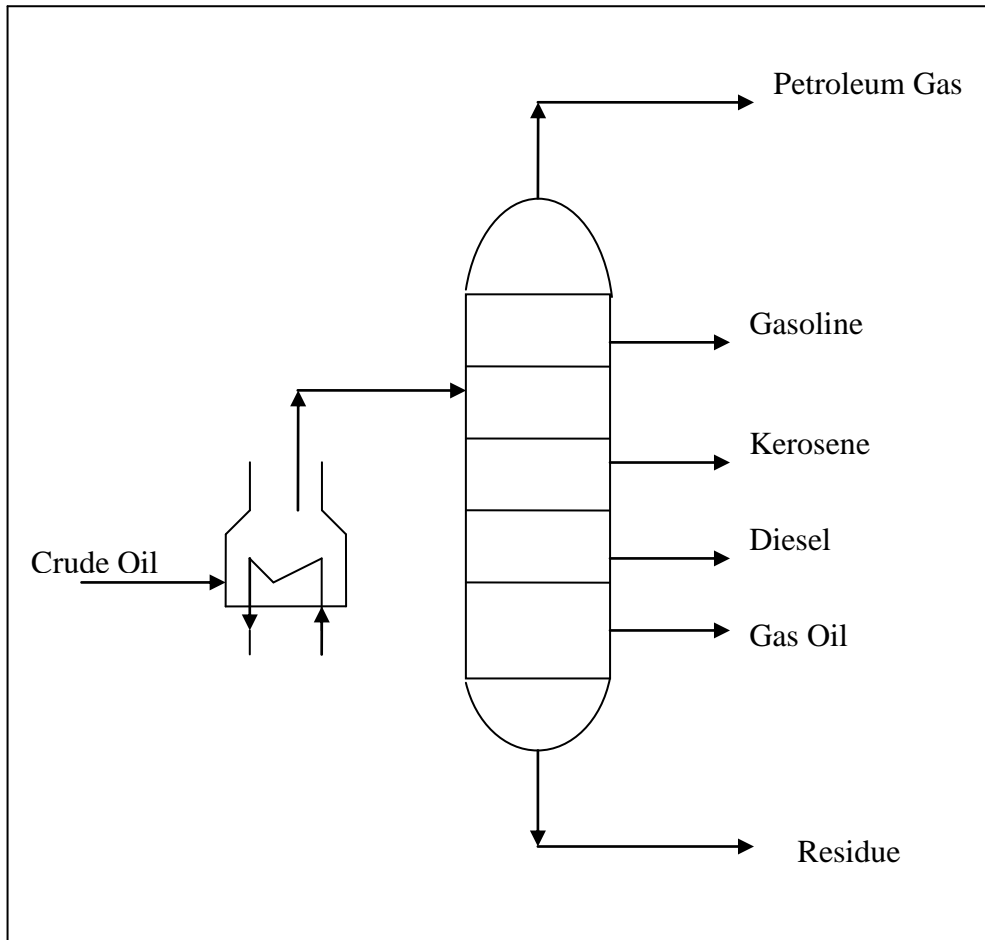
This configuration continuously takes a feed and separates into products as shown in *Figure 2.1*. Liquid runs down the column due to gravity, while the vapour runs up the column. The column section above the feed tray rectifies the vapour stream with light

components and therefore is termed as rectifying section (Gary and Handwerk, 1984). The column section below the feed tray strips heavy components from the vapour streams to the liquid stream and is termed as stripping section.



**Figure 2.1:** Continuous Distillation Column

Continuous distillation is used widely where large quantities of liquid have to be distilled. It finds its widest application in petroleum refineries. In refineries, the crude oil feedstock is separated into their fractions, e.g. light gases, naphtha, diesel, etc. in a multiple product tower (*Figure 2.2*)



*Figure 2.2: Crude Oil Distillation Column*

### **2.3 Batch Distillation Column**

Batch distillation is, perhaps the oldest operation used for separation of liquid mixtures. For centuries and also today, batch distillation is widely used for the production of fine chemical and specialised products such as beverages, essential oils, perfume, pharmaceutical and petroleum products.

In batch distillation, as the overhead composition varies during operation, a number of main-cuts and off-cuts are made at the end of various distillation tasks or periods. Purities

of the main-cuts are usually determined by the market or downstream process requirements but the amounts recovered must be selected based on the economic trade off between longer distillation times (hence productivity), reflux ratio levels (hence energy costs), product values, etc. Increasing the recovery of a particular species in a particular cut may have strong effects on the recovery of other species in subsequent cuts or, in fact, on the ability to achieve at all the required purity specifications in subsequent cuts. The profitable operation of such processes therefore requires consideration of the whole (multiperiod) operation Mujtaba, (2004).

Batch distillation columns offer greater flexibility with respect to variations of feed mixtures, feed composition, relative volatilities and product specification, and plays an important role in the chemical process industries and typically used, where,

1. The compositions of the materials vary over wide range.
2. The separation only needs to be performed infrequently, such as pilot-plant operation.
3. The materials to be separated are produced in relatively small quantities, such as in small scale commercial facilities.
4. The main product contains only relatively small amounts of light and/or heavy impurities.

Selection of batch distillation usually involves evaluating the performance of an existing distillation system to determine whether its performance is acceptable. However, it may be necessary to design a new system for specific separation to be performed.

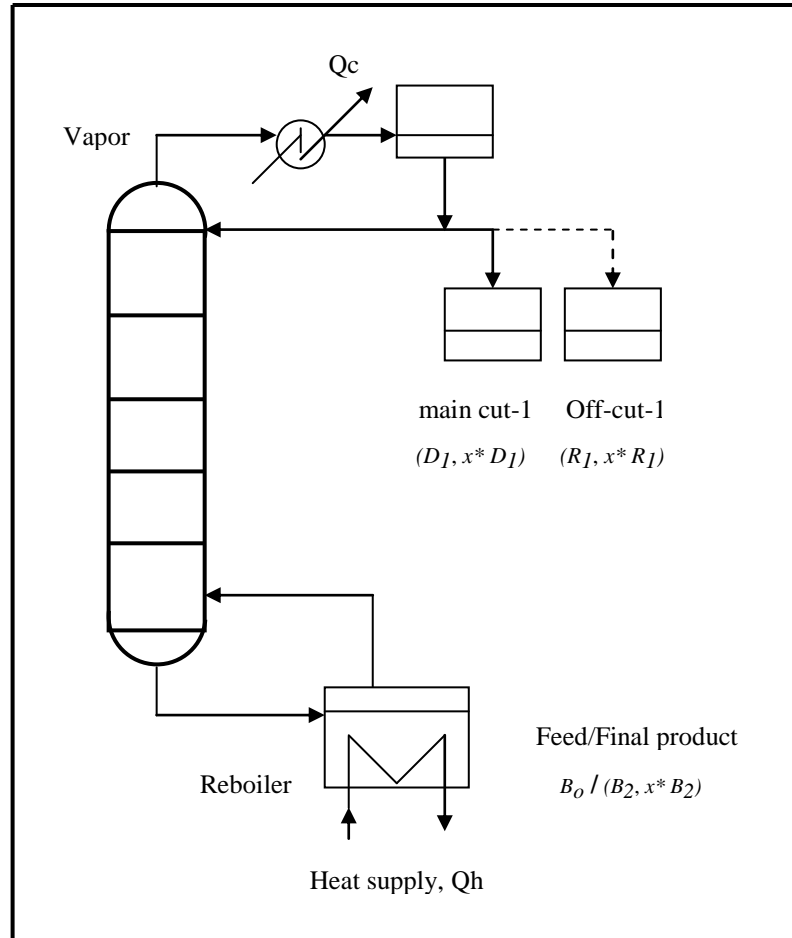
There are two major types of batch distillation columns, each one designed to perform specific types of separations, and these types are; conventional and unconventional batch distillation column.

## **2.4 Conventional Batch Distillation (CBD)**

In this configuration as shown in a schematic diagram (*Figure 2.3*), the available separation section (tray or packed) is utilised in rectifying mode, with product cuts (recovered) and intermediate off-cut fractions (disposed of or recycled) collected as condensed distillate. A final residue bottom fraction may also be a desired product.

The conventional batch distillation consists of a reboiler, a rectifying column (tray or packed), and a series of product accumulator tanks connected to the product streams to collect the main and intermediate fractions.

In this column, the charge is loaded into the reboiler at the beginning of the process and heated to its boiling point. Vapour flows upwards in the column and condenses at the top. After some time, a part of the overhead condensate is withdrawn continuously as distillate, and the other part is returned to the column section as reflux. The liquid in the reboiler is increasingly depleted of more volatile components. As the amount of liquid in the reboiler decreases, the concentration of high boiling constituents increases.



**Figure 2.3:** Conventional Batch Distillation Column (CBD)

More than one batch is considered in a long-term production campaign if the total amount of mixture to be processed is more than the capacity of the column. During processing a particular batch, as the overhead composition varies (*Figure 2.4*) Mujtaba (2004), a number of main-cuts and off-cuts are made at the end of various distillation tasks. In campaign mode, each intermediate off-cut may be collected and stored separately and fed to the reboiler sequentially and reprocessed in subsequent batches (Luyben *et al*, 1990; Mujtaba and Macchietto, 1992a). The other alternative is to collect and store each off-cut separately

for sometime and reprocessed when the amount of material of each off-cut reaches to the level of one full batch charge (Mujtaba and Macchietto, 1994).

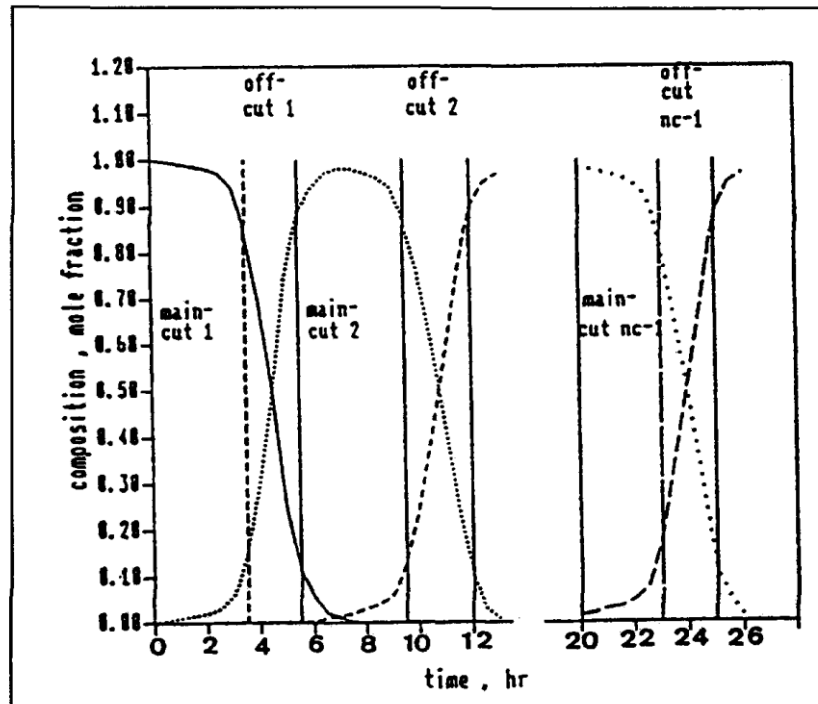


Figure 2.4: Typical Instant Distillate Composition Profile (Mujtaba, 2004)

Logsdon *et al.* (1990) presented a simultaneous optimization strategy for the design and operation of batch distillation columns undergoing both single and multiple separation duties defined in Mujtaba and Macchietto (1996). They defined an objective function in terms of net profit, which was maximized during optimization. They optimized the number of stages and column operation policy (reflux ratio, batch time). Optimal design (vapour load,  $V$  and number of stages  $N$ ) and operation (reflux,  $r$  and batch time,  $t_b$ ) of batch distillation have received significant attention Al- Tuwaim and Luyben (1991), Diwekar *et al.* (1989), Logsdon *e al.* (1990), Mujtaba and Macchietto (1996), Sharif *et al.* (1998) and Hasebe *et al.* (1995).

Diwekar *et al.* (1989) introduced a shortcut method for optimal design of single and multiple fraction batch columns operating under constant and variable reflux condition. They investigated the effect of design parameters of the column ( $N$  and  $V$ ) on an economic objective function (annual profit). It was suggested that  $V$  should always be at its maximum value (design value) to give the maximum profit. In the other words,  $V$  should be greater than zero but can have any value.

## **2.5 Non Conventional Batch Distillation Methods**

Alternative configurations, collectively identified as non conventional columns, have been found in certain cases to be more advantageous. Three among them will be reviewed in this section:

2.5.1 Inverted Batch Distillation Column (*IBD*).

2.5.2 Middle Vessel Batch Distillation Column (*MVBD*).

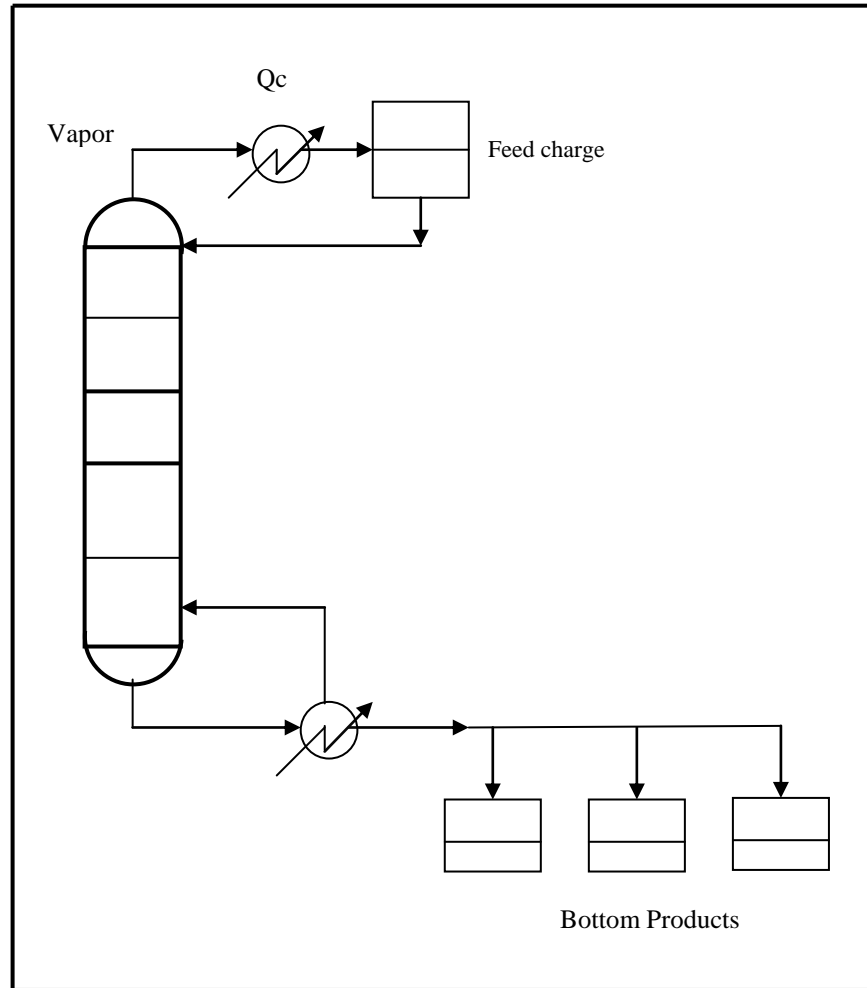
2.5.3 Multivessel Batch Distillation Column (*MultiVBD*).

### **2.5.1 Inverted Batch Distillation Column (*IBD*)**

This type of batch distillation column (*Figure 2.5*) was originally proposed by Robinson and Gilliland (1950). In the inverted column, the feed is charged to the condenser drum. The liquid flowing down the column is vaporised in the reboiler and a fraction is removed as product accumulator. The products are taken out sequentially, the heaviest component first, then the second heaviest, etc.

This type of column operates exactly as the conventional batch column except that products are withdrawn from the bottom. High boiling (heavy components) products are withdrawn

first followed by the more volatile products. This type of operation is supposed to eliminate the thermal decomposition problem of the high boiling products.



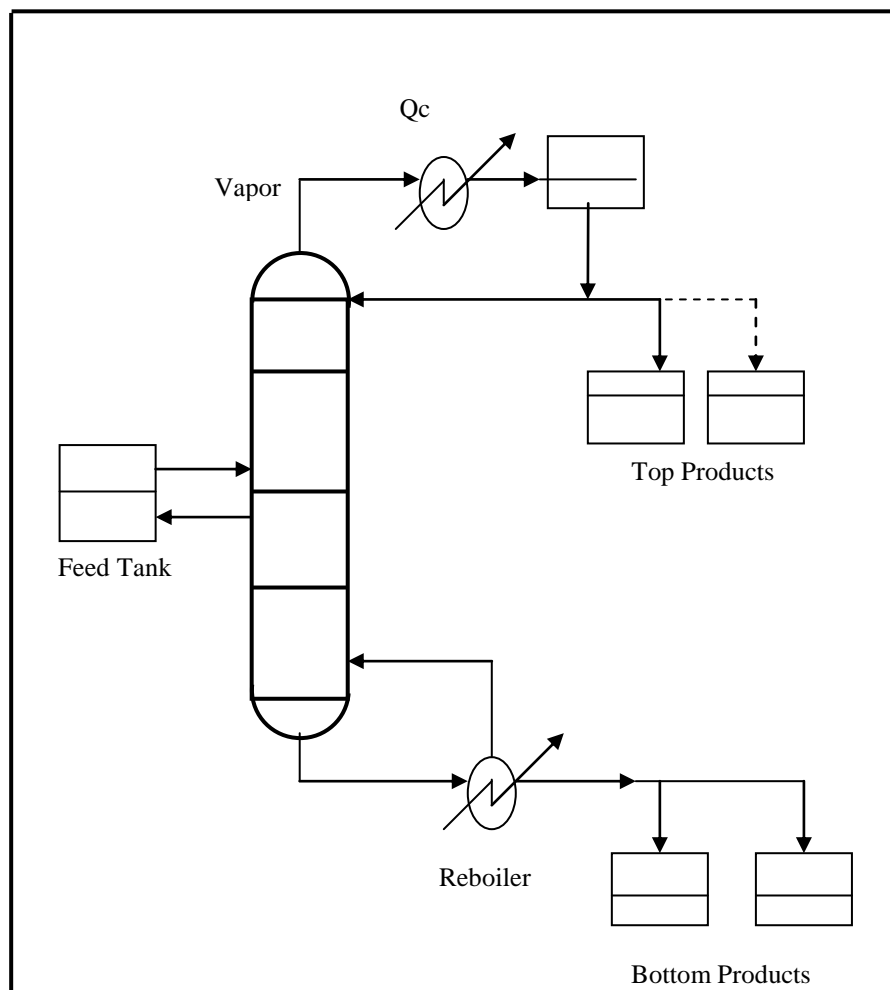
**Figure 2.5:** Inverted Batch Distillation Column (*IBD*)

Abrams *et al.* (1987), Mujtaba and Macchietto (1994), and Sorensen and Skogestad (1996) considered such columns for batch distillation and compared their performances with conventional columns.

## 2.5.2 Middle Vessel Batch Distillation Column (MVBD)

The second type is a combination between both conventional and inverted operations which means the middle vessel batch distillation as shown in (Figure 2.5), simultaneously taking the lighter components overhead and the heavier components out of the bottom with the reservoir in between.

Bortolini and Guarise (1970) present such columns and methods for evaluating their performance with binary mixtures.



**Figure 2.6:** Middle Vessel Batch Distillation Column (MVBD)

Recently, the use of such columns has been considered by Hasebe *et al.* (1992), Mujtaba and Macchietto (1994), Barolo *et al.* (1996-a, b and 1998), Zamprogna *et al.* (2001), Greaves *et al.* (2003), and Safrit and Westerberg (1997) for nonideal, azeotropic, extraction and reactive separation of binary and multicomponent mixtures. This type of column is inherently very flexible in the sense that it can be easily converted to a conventional or inverted batch distillation column by changing the location of the feed and by closing or opening appropriate valves in the product lines.

### **2.5.3 Multivessel Batch Distillation Column (*MultiVBD*)**

The third type is known as a Multivessel batch distillation column *MultiVBD* column, and has very similar configuration of that of a conventional batch distillation but with one or more intermediate charge/product vessels which is connected with the columns as shown in *Figure 2.7*, which consists of a reboiler, two intermediate vessels, a condenser vessel and three column sections.

If the column operates at total reflux, the charges in each vessel will be purified as the distillation proceeds. However, the purity in each vessel will depend on the number of plates in each section of the column, vapour boil-up, the amount of initial charge in each vessel and the duration of operation. The top vessel will be richer in low boiling components while the bottom vessel will be richer in high boiling components. However, the researches in this area are fairly handful and all investigations were concerned with only quarterly mixtures and without (off-cut) fractions.

One configuration of particular interest in this study is Multivessel batch distillation column, which can be viewed as a generalization of all previously studied batch column configuration. The Multivessel system is a novel batch distillation configuration that offers improved separation performance compared to the conventional single-column batch rectifier.

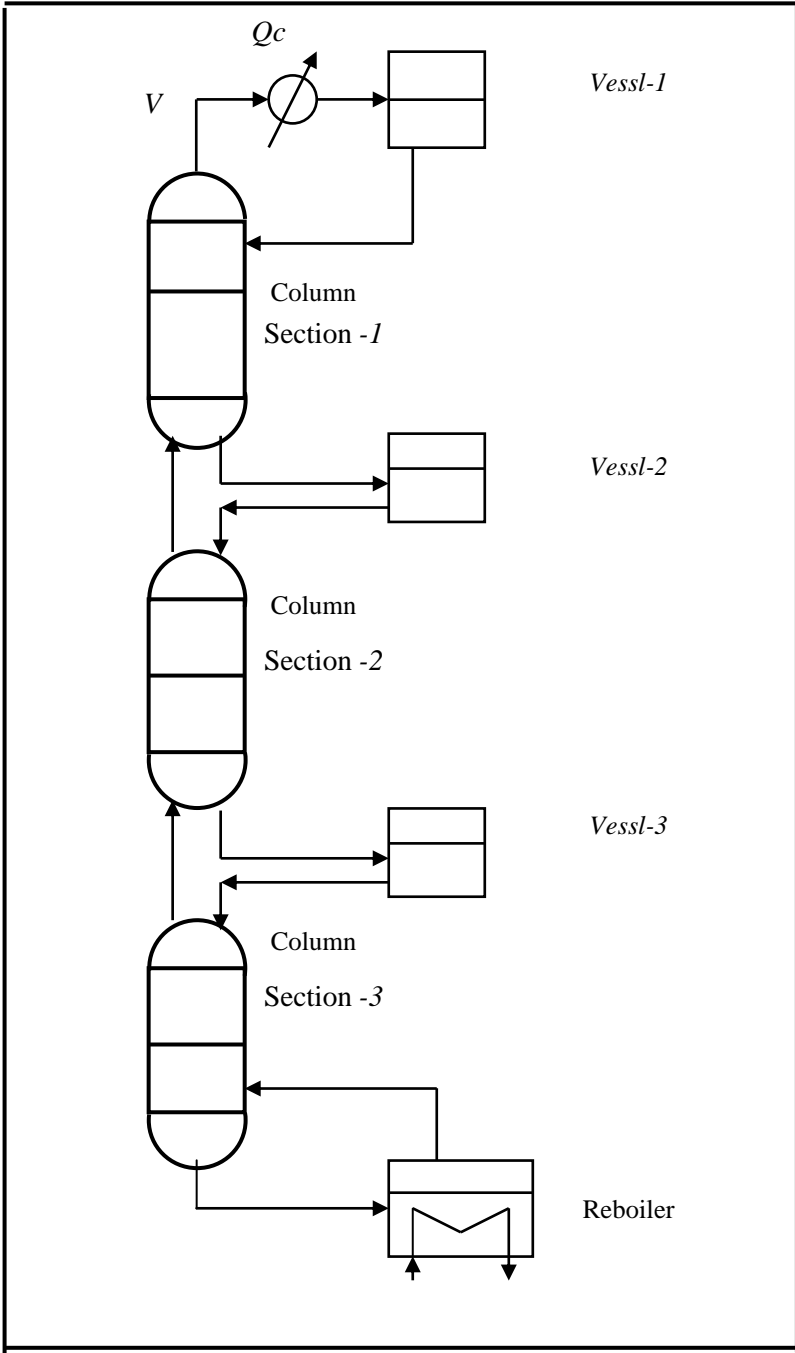


Figure 2.7: Multivessel Batch Distillation Column (MultiVBD)

This thesis is focused on the optimal design and operation of *MultiVBD* with different column sections for binary and ternary distillation under fixed product demand (in terms of number of batches) and strict product specification. Both the vapour load and number of stages in each column section are optimised to maximise a profit function. The performance of *MultiVBD* is compared with the performance of *CBD* on respect to the net profit ( $P$ ). Also in this work, the effect of different separation tasks on the optimum design and operation for ternary batch distillation is considered to show the improvement in overall profitability. There are limited studies that used the *MultiVBD*, for simulation, control and optimisation studies, for example, Hasebe *et al.* (1995), Wittgens *et al.* (1996), Furlonge *et al.* (1999), Low and Sorensen (2003, 2004, and 2005) and Ruiz and Luiz, (2006).

There are several studies that compare the optimal operation of the *MultiVBD* system to that of the traditional regular column system *CBD* (Low and Sorensen *et al.*, 2003; 2004 and 2005) The performance indexes used for the comparison included maximum production rate and minimum mean energy consumption.

The *MultiVBD* system was first proposed by Hasebe *et al.* (1995) whereby the concepts of the inverted column and middle-vessel column by Robinson and Gilliland (1950) were extended to what they termed as the multi-effect or *Multivessel* distillation system. Since then, the *Multivessel* system has been shown, both via simulation and experimental studies, to offer a better performance than the conventional regular-column system with the same number of stages.

Wittgens *et al.* (1996) considered *MultiVBD* column and proposed a generalization of previously batch distillation schemes. A simple feedback control strategy for total reflux

operation of a *MultiVBD* column is used. The feasibility of their strategy is demonstrated by simulations. An experimental column based on the proposed control scheme has been built and the experiments verify their simulations.

Furlonge *et al.* (1999) presented a *MultiVBD* column and proposed the optimal operation problem for a fixed number of stages (total and in between the vessels). The objective was to minimise the mean rate of energy consumption required for producing products of specified purity while optimizing instantaneous heat input to the reboiler subject to product specifications (amount and purity). Various operating policies such as fixed vessel holdup, variable vessel holdup, etc. have been considered. Optimising the initial distribution of the feed among the vessels reduces the energy consumption by almost 15%.

Low and Sorenson (2005) considered the optimal configuration, design and operation of batch distillation column based on overall profitability for a given separation duty. Using rigorous model, the mixed integer dynamic optimisation problem was solved using genetic algorithm. Again for a multicomponent separation case, *MultiVBD* configuration was chosen as optimum from among the conventional and inverted batch distillation columns. They compared the performance of *MultiVBD* with that of *CBD* and found that the *MultiVBD* is more profitable than in *CBD*. However, strict product specification was not maintained and the vapour load hit the upper bound to minimise the batch time and to maximize the profit.

There is no much literature in this particular area (*MultiVBD*), nevertheless extensive research is done on the operation of conventional batch distillation columns. Some of these research activities for (*MultiVBD*) are focused on the optimization of the reflux flow to the

column to either keep the top product composition constant or minimise energy consumption.

The *MultiVBD* column is useful for the separation of multicomponent mixtures frequently found in the chemical process industries. Hasebe *et al* (1995) indicates that the energy efficiency of a Multivessel batch distillation could be comparable to continuous distillation. Although batch distillation generally is less energy efficient than continuous distillation, it has received increased attention in the last few years because of its simplicity of operation, flexibility and lower capital cost.

Hasebe *et al.* (1999) attempted to compare the operation of the *MultiVBD* with the continuous distillation column. They used performance index for the *MultiVBD* (production rate divided by vapor flow rate) and the continuous distillation column (sum of product flow rates divided by the sum of vapor flow rates), and found that the separation performance of the *MultiVBD* is comparable to the continuous process from the point of view of energy consumption.

Several control strategies for the *MultiVBD* have been proposed. (Wittgens *et al.*, 1996) proposed a feedback control structure based on temperature controllers. The idea is to adjust the reflux flow out of each of the upper vessels location in the column section below. There is no explicit level control rather the holdup in each vessel is adjusted indirectly by varying the reflux flow to meet the temperature specifications. Their simulation results indicate that the temperature controller achieved the same steady state product composition in the vessels that is independent of initial feed composition, thus able to tackle feed composition distributions. Also, their study proposed implementation of the multivessel

batch distillation column via pilot plant experimental setup. The experimental results confirmed the results from the simulations.

Noda *et al.* (2000) later presented a more complex on-line feedback-control strategy to optimally operate the *MultiVBD*. The on-line system consists of four subsystems, namely a composition measuring subsystem using a near-infrared analyzer, composition estimation and model update subsystem, an optimisation subsystem, and, finally a control subsystem.

Low and Sorenson (2003, 2005) presented the optimal design and operation of *MultiVBD* column. A profit function based on revenue, capital cost and operating cost was maximised while optimising the number of stages in different column sections, reflux ratio, etc. They compared the performance of *MultiVBD* with that of conventional batch distillation column for a number of different mixtures.

## **2.6 Total Reflux Operating Policies for *MultiVBD* Column**

The simplest strategy for operating the *MultiVBD* column which is focused in this work, the *total reflux* operation suggested by Hasebe et al, (1995), where the product rates are set to zero. In the simulation the initial time was considered at ( $t= 0$ ) and the initial composition in all vessels is equal to that of the feed mixtures. Their scheme involving the optimisation of the vessel holdups and their adjustment based on composition measurement in these vessels, is rather complicated to implement and it requires an advanced control structure to implement the control law. There are four different operating policies for *MultiVBD*; these differ in the initial distribution of the feed, and they are:

### **Policy 1- Constant holdup**

In this policy the feed is distributed among the reboiler, intermediate vessels, and reflux drum. All these holdups are kept constant throughout the operation which takes place under *total reflux*.

### **Policy 2- Optimal holdup**

The holdups in the reboiler, side vessels and reflux drum are allowed to vary. The feed either is charged wholly to the reboiler or is optimally located and the column is operated at *total reflux*.

### **Policy 3- Optimal product withdrawal**

This policy unlike the previous policies 1 and 2, where liquid (product) allowed to withdrawn from reflux drum and side vessels during the operation since this policy allows the option of holding the vessel holdups constant or having no product withdrawal.

### **Policy 4- Feed back control**

A feedback control strategy proposed by Wittgens *el al*, (1996) is employed, where the reflux flowrates was adjusted based on temperature measurements on the middle of tray of each column section. The controller gains and the temperature set- points are optimised.

In this work, the constant holdup is used (fixing amount of each product) and the holdup of each vessel for *MultiVBD* column is calculated in advance by taking into account the amount of feed, feed composition and product specifications. After feeding the predescribed amount of raw material to the reboiler, vessels and reflux drum, the total reflux operation with constant vessel holdup is carried out until the product specifications are achieved or until the improvement in product purity.

In the simulations the initial time was considered (at  $t = 0$ ) and the initial composition in all vessels is equal to that of the feed mixture. In all simulations, the vapor flow is kept constant.

Hasebe *et al.* (1995), proposed to “control” the total reflux *MultiVBD* batch distillation column by calculating in advance the final holdup in each vessel and then using a level control system to keep the holdup in each vessel constant. For cases where the feed composition is not known exactly they propose to, after a certain time, adjust the holdup in each vessel based on composition measurements. Their scheme, involving the optimization of the vessel holdups and their adjustment based on composition measurement in these vessels, is rather complicated to implement and it requires an advanced control structure to implement the control law.

Sorensen and Skogestad (1996) found the total reflux operation to be better for separations with a small amount of light components. Here, the operation is switched between total reflux operations and dumping of the product (*i.e.* the condenser holdup is introduced as an additional degree of freedom).

## **2.7 Conclusions**

Different types of unconventional batch distillation column used in the past and conventional batch distillation, are generally considered in the literature. Also in this chapter a general reviews on distillation column are considered and discussed. Brief

description is given for total reflux operating policies of MultiVBD column with constant vessel holdup of *MultiVBD* column.

From the previous literature review in this chapter, the studies have demonstrated that the *MultiVBD* column is more profitable than in *CBD* column and useful for the separation of multicomponent mixtures frequently found in the chemical process industries (Low and Sorenson, 2003; 2004 and 2005).

# CHAPTER 3

## PROCESS MODELLING AND OPTIMISATION

### 3.1 Introduction

This chapter highlights the reviews of the past work on process modelling, and process optimisation of multivessel batch distillation column. The gPROMS software is the main tool for modelling, simulation and optimisation used in this thesis, the main features of the software is presented with the operating procedures of software such as MODEL, PROCESS, and OPTIMISATION sections. Also an overview of some papers considering modelling, simulation and optimisation of *MultiVBD* column are presented.

### 3.2 Process Modelling

Process models are very useful. They can be used for operator training; safety analysis and design of safety systems; process design and process control systems design. The development of faster computer and sophisticated numerical methods has enabled modelling and solution of complete systems (process), while in the past one had to separate the system to its constituent parts “Mathematical modelling” of system or (process) concerns with quantitative rather than a qualitative treatment of the process.

Modelling and simulation can bring the following advantages:

- 1- Process understanding can be improved.
- 2- Operating policies can be optimized.
- 3- The number of test runs to be performed on the plant is kept to a minimum, which improves safety and saves money.
- 4- Plant personnel can be trained directly on the model rather than on the plant. Using a model is cheaper than using the real process.
- 5- It is less time consuming.
- 6- It is safer, and the outcome is much less fatal if something goes wrong with the study.

Often when engineers analyze a system to be controlled or optimised, they use a mathematical model. In analysis, engineers can build a descriptive model of the system as a hypothesis of how the system could work, or try to estimate how an unforeseeable event could affect the system. Similarly, in control of a system, engineers can try out different control approaches in simulations.

A mathematical model usually describes a system by a set of variable and a set of equations. The mathematical equations are to study the dynamic of a real system. Mathematical models are used particularly in the natural sciences and engineering disciplines such as physics, biology, and electrical engineering, but also in the social sciences such as economics, sociology and the political science; physicists, engineers, computers scientists, and economists use mathematical models most extensively.

The values of the variable can be practically anything; real or integer number, Boolean values or strings, for example. The variables represent some properties of the system, for

example, measured system outputs often in the form of signals, timing data, counters, event occurrence (yes/no). The actual model is the set of functions that described the relations between the different variables. Over the last thirty years the identification problem became an essential area of study for model theory. A mathematical model uses mathematical language to describe a system.

Eykhof (1974) defined a mathematical model as a representation of the essential aspects of an existing system or a system to be constructed with present knowledge of that system in usable. However, for many complex chemical processes, the models results in a set of non-linear equations requiring numerical solution.

In recent years, (Mujtaba, 2004) mentioned that the choice in many cases depends on the numerical techniques available for the solution of the equations. The models have to be in place and give a fair representation of the system to be studied. Modelling batch distillation systems were the main interest area of many researchers in the past (Diwekar *et al.*, 1995; Nad and Spiegel, 1987; Mujtaba, 1989, 1992, 1997; lang *et al.*, 1994).

### **3.3 Process Simulation**

Simulation is defined as the study of a process or is the imitation of some real thing, state of affairs. The act of simulating something generally entails representing certain key characteristics or behaviours of a selected physical or abstract system. Franks, (1972) recognises general levels of simulation. Obviously this is feasible to estimate error bounds in a number of situations. Simulation is used in many contexts, including the modelling of

natural systems or human systems in order to gain insight into their functioning. Other contexts include simulation of technology for performance optimization, safety engineering, testing, training and education

A great deal of mathematical skill and effort is required to solve even some of the simplest of non-linear equations and such level is usually beyond the reach of the average process engineer.

Many different types of software packages are available in the market. Modern tools are numerically powerful, highly interactive and allow sophisticated type of graphical and numerical output. This allows a user to develop a competitive advantage by representing their own processes. They also allow optimisation and parameter estimation.

Chemical process simulators simplify the process of evaluating the different design alternative without the need of making too much process assumptions and considering the entire process structure (Teresa *et al.*, 2003). A process simulator has the capability to input and modify the configuration of the process flowsheet and to perform design calculations considering the complete process flowsheet, before they are tried on the actual plant. In this way, it is possible to model and predict the behaviour of the process flow sheet and to study different operation scenarios (e.g. higher flow rates, different feedstock, modified operating conditions, various levels of energy integration, etc.) in combination with evaluations of the process economics and potential environmental impacts.

Process simulation is an engineering tool for the design and optimisation of steady state and dynamic chemical process. Process simulation offers many benefits. It is much easier to

incorporate actual process data into a simulation model instead of building a pilot plant and its economics.

### 3.4 Process Optimisation

The mathematical optimisation is the branch of computational science that seeks to answer the equation ‘What is best?’ for problems in which the quality of any answer can be expected as a numerical values. Such problems arise in all areas of business, physical, chemical and biological science, engineering, architecture, economics, and management.

Optimization provides a complete range of techniques from the basic multiple run approach of trial and error to highly complex numerical strategies. A benefit of optimisation would include improved product yield, conversion, productivity, profit or operating time.

Batch distillation is a dynamic process. The determination of optimal control strategy with respect to a maximal gain in the products and minimal production time is one of the main goals in the design and operation of the production processes (Perkins and Walsh, 1996).

The optimisation problem to optimise the operation of *CBD* and *MultiVBD* column can be stated as follows:

*Objective function:* the quantity we need to optimise (maximum or minimum).

*Control variables:* the parameters, which may change in the search for the optimum

*Constraints:* the restrictions allowed on parameters values.

Mathematically it can be represented as:

*OP*                      Minimise or (Maximise)              J (Objective function)



### **3.5 Modelling and Simulation of Multivessel Batch Distillation**

In this thesis, the Multivessel batch distillation column is considered with the total reflux operation which is suggested by Hasebe *et al.* (1995).

Simulating the actual operation of *MultiVBD* has been studied in the last few years, but with less attention compared to conventional distillation. Simulation is an imitation of some real thing, state of affairs, or process. The main interest was usually to develop models that could be best predicting the operation of the column with the development of high speed digital computers. In this chapter the review of the past work on the modelling, simulation and optimisation of Multivessel batch distillation column is presented.

gPROMS software is the main simulator used for modelling, simulation and optimisation. It allows simulation with different models. The main features of the software will also be briefly discussed here in this chapter.

Skogestad *et al.* (1997) simulated a *MultiVBD* column with simple model based on constant relative volatility and constant molar liquid holdup on the stages, total condenser and constant pressure using a total reflux operation. Robinso (1970); Luyben (1988); Mujtaba and Macchietto (1992) used this mode for simulation and optimisation of conventional batch distillation.

### **3.6 Optimisation Studies of *MultiVBD* Batch Distillation**

The optimisation of *MultiVBD* column is generally considered in the literature as optimal operation problem.

Normally, the problems in engineering process design or plant operation have many, and possibly an infinite number of solutions. Optimisation provides a complete range of techniques from the basic multiple run approach of trial and error to highly complex numerical strategies.

A benefit of optimisation would include: improve product yield, conversion, productivity, profit or operating time. There are many ways optimisation techniques and decisions come into play when applied to the design and operation of chemical processes and plants. Some of them can be stated as follows (Ekpo, 2006):

- Determination the best sites to locate a process.
- Optimum pipeline sizing and layout.
- The entire design of the plant, as well as the “best” location for each piece of equipment.
- Plant operation for maximum productivity and profit.
- Bloated inventories are a major cause of inefficient operations optimisation can help in the slashing or minimisation of inventory costs.

Low and Sorenson (2003) presented the optimal design and operation of *MultiVBD* column. A profit function based on revenue, capital cost and operating cost was maximized while optimising the number of stages in different column sections, reflux ratio, etc.

Low and Sorenson (2004) considered the optimal design and operation of *MultiVBD* and other configurations. Several design case studies are presented and a comparison of optimal designs for various design scenarios, such as different production time, capital costs, process allocation, and mixture characteristics. The optimisation problems were to minimise the energy consumption and to optimise the number of trays and vapour rate for

different mixtures. Also they used three different batch distillation models of complexity in their studies (simple, detailed, and rigorous models). The objective function was to maximise the profit.

Low and Sorenson (2005) considered the optimal configuration, design and operation of batch distillation column based on overall profitability for a given separation duty. Using rigorous model, the mixed integer dynamic optimisation problem was solved using genetic algorithm. Most of the earlier studies on the optimization of *MultiVBD* column employed different models. *Table 3.1* summarise the past work on dynamic optimisation of *MultiVBD* column.

**Table 3.1:** Summary of the Past Work on Optimisation of *MultiVBD* Column

Reference	Column Type	Model Type	Mixture	Off-cut	Objective Function
Furlong <i>et al</i> (1999)	MultiVBD	Rigorous	Multicomponent	–	Minimum Energy
Low and Sorenson (2003)	MultiVBD CBD	Detailed and Rigorous	Multicomponent	–	Maximum Profit
Low and Sorenson (2004)	MultiVBD CBD	Simple, Detailed, Rigorous	Multicomponent	–	Maximum Profit
Low and Sorenson (2005)	MultiVBD CBD, Inverted BD	Rigorous	Binary and Multicomponent	–	Maximum Profit
Luiz and Ruiz (2006)	MultiVBD	Simple	Multicomponent	–	Maximum Profit
This work & Mahmud <i>et al</i> (2008)	MultiVBD	Simple	Binary and Multicomponent	Off-cut	Maximum Profit

### 3.7 Process Simulator

A general purpose simulator has wide application in process industry. These packages often have sophisticated languages and formalisms for model development that allow the description of complex differential/algebraic models.

Steady state process simulators make it possible to run the plant as a model on a computer and test out operation scenarios (*e.g.* higher flow rates, different feedstock, modified operating conditions, etc.) before they are tried on the actual plant.

Examples of commercially available process simulators that can be used to model chemical processes are ASPEN PLUS™ and HYSYS™ by Aspen Technology Inc., CHEMCAD™ by ChemStations, Inc., gPROMS by Process Systems Enterprise Ltd., and PRO/II by Simulation Sciences Inc., etc.

With the ever-increasing capabilities in computer power and accurate models for describing process units, process simulators make it possible to do rigorous analyses and exploring different design alternatives. In addition to the classical experimental approaches (*e.g.* bench scale, mini-plant, pilot plant, market development plant), the use of modelling and simulation tools is becoming increasingly popular and powerful.

Also there are many specific modelling packages that can be used to simulate some process. In general simulators can be classified in two categories: specific and general packages. Specific packages require and give detailed information and it could be used only for the process for which it is developed. While the general one is used for any process in the following a number of simulators will be discussed.

### **3.7.1 gPROMS Simulator**

The gPROMS (**g**eneral **P**rocess **M**odelling **S**ystem) package is an equation oriented general propose modelling, simulation and optimisation tool for combined discrete and continuous process, which makes it particularly suitable for the modelling and simulation of any plant operation (steady state and dynamic).

gPROMS as modelling tools allows direct mathematical description of distributed unit operations chemical processes. gPROMS task language makes a clear distinction between the model of a system and specifics of the activities in which this model may subsequently be employed. gPROMS has a wide range of application and it can be used for steady state and dynamic simulation. It can also be used to reform parameter estimation calculations for complex process under both conditions. It is extremely helpful for continuous processes that often exhibit transient behaviour either due to abnormal condition. gPROMS was developed by Process System Enterprise, based at Imperial college of London and has been widely used for industrial processes such as batch plant (Winkel *et al.*, 1995).

gPROMS license is more flexible for the our company in Libya which allows us to use the particular package gPROMS program without buying the full software packages.

### **3.7.2 Feature of gPROMS**

Many different types of software packages are available in the market. Modern tools are numerically powerful, highly interactive and allow sophisticated types of graphical and numerical output. Here the conventional and unconventional batch distillation configuration processes considered in this thesis and modelled and optimised using the software package

“general Process Modelling System” (gPROMS) developed by Process Systems Enterprise Ltd., London.

A single gPROMS model of a process can perform many activities, such as:

- 1) Laboratory experiment design and optimisation
- 2) Detailed design of the complex unit
- 3) Simultaneous optimisation
- 4) Detailed design and optimisation
- 5) Design of optimal procedures

Moreover, it has a built-in to MS Excel that allows the user to automatically test the statistical significance of results, generate plots overlaying model data and experimental data, plot confidence ellipsoids.

gPROMS has many advantages that make it an attractive tool for solving dynamic and steady state modelling problems. All of the complexity of the underlying equations and their solution of dynamic or steady state simulation, optimisation, or parameter estimation are hidden from the user. It also is an open source software structure. It can easily link to external components, for example, physical properties packages or control system software different model. It allows simultaneous optimisation of equipment sizes and operating procedures that saves capital and operational costs in long run.

### 3.8 Defining a Task/Process/Optimisation

In gPROMS software, the TASK and MODEL are defined as the modelling of operating procedures and control strategies,

The PROCESS is analysed by the composition of different levels of Models in hierarchical order.

The TASK/PROCESS is:

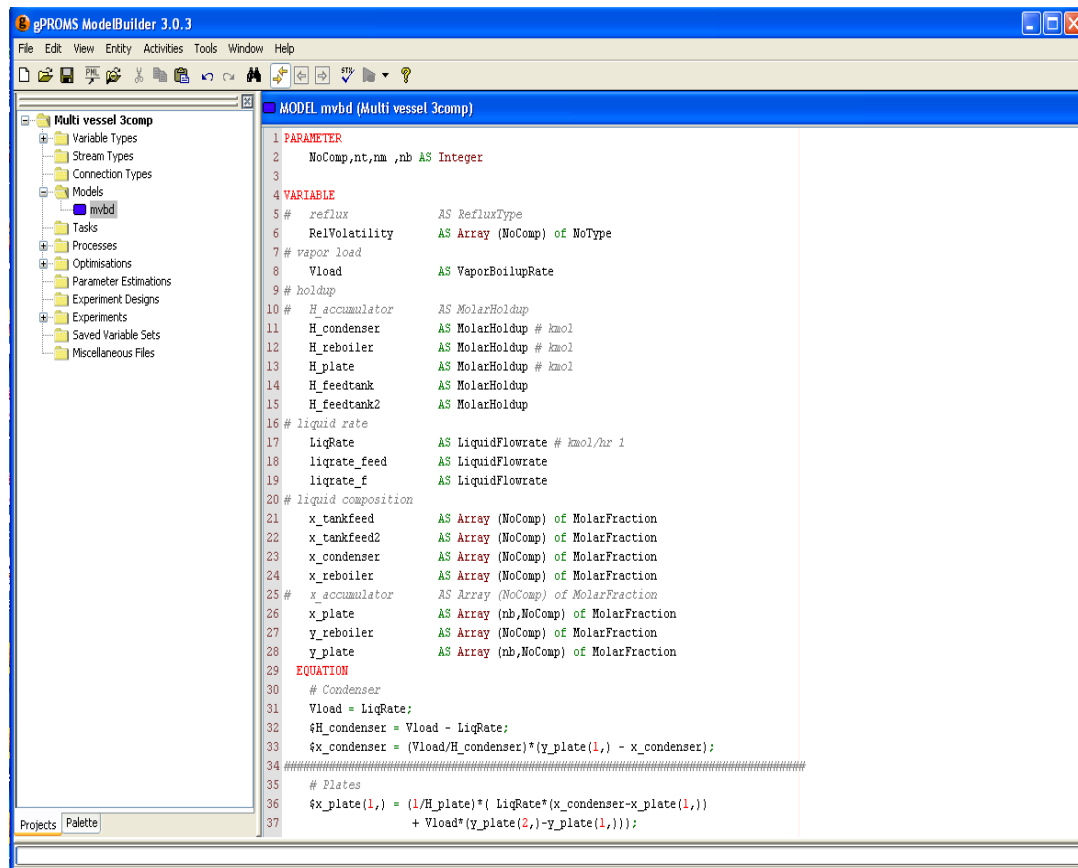
- What to do?
- How to do it?
- When to do it?

The TASKS are used in the PROCESS to define individual operating procedures.

The model entity is general information needs to be specified in any MODEL is described in the following:

- A set of constant parameters that clarify the system. They are declared in the PARAMETER section.
- A set of variable that describe the time-dependent behaviour of the system. They are declared in the VARIABLE section.
- A set of equations involving the stated variable and parameters. They are declared in the EQUATION section.

Model equations for batch distillation column are modelled within g PROMS model builder and shown in (*Figure 3.1*).



The Processes (contains specification for simulation the batch column). It is separated into sections that contain information necessary to define a dynamic simulation activity. The main process sections used to carry out simulation studies in this work are:

- Unit
- Set
- Assign
- Initial
- Solution parameters
- Schedule

The Screenshot of entity PROCESS for dynamic simulation involving the batch distillation process is shown in (Figure 3.2)

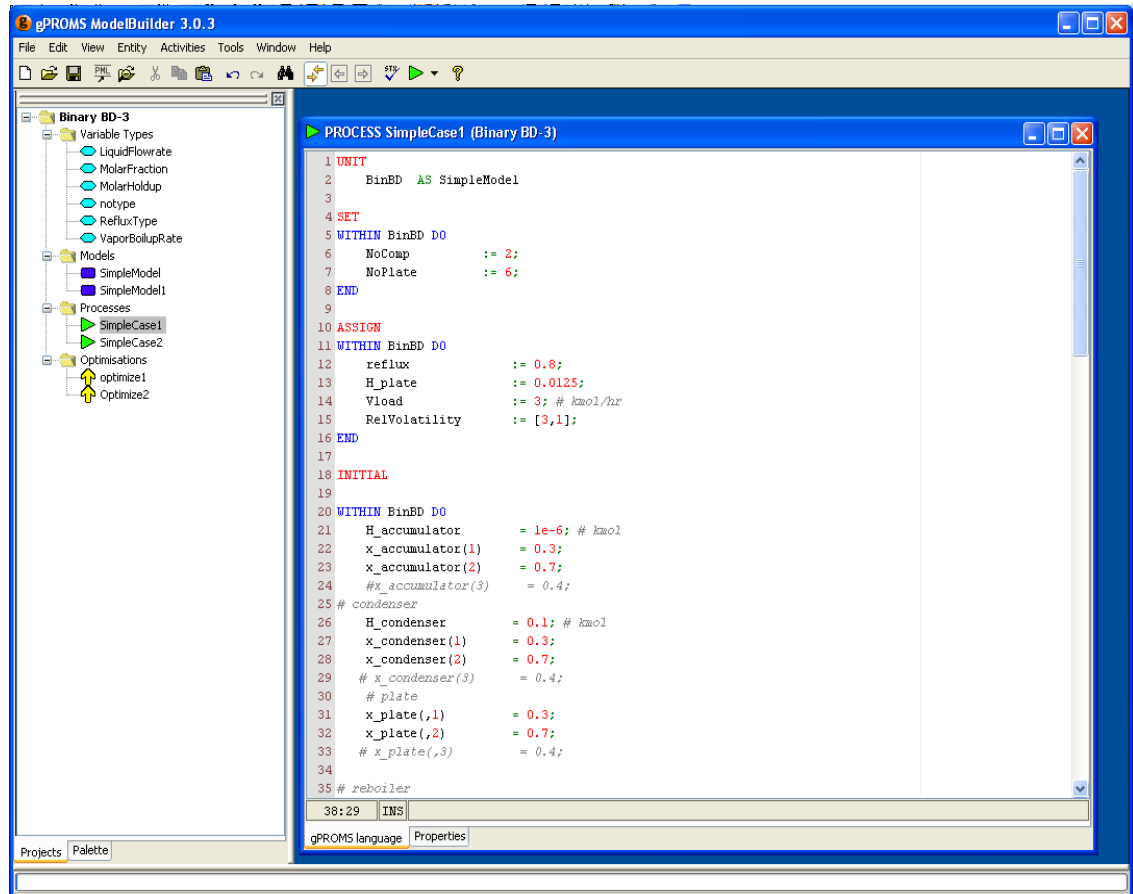


Figure 3.2 An Overview of the gPROMS (Part of the Processes File)

In The optimisation entry, the parameters for dynamic optimisation problems are specified in many cases, the values are expresses in the form: [guessed value, lower bound, upper bound] and it has three additional tabs to formulate the optimisation problem quickly as shown in (Figure 3.3), and they are:

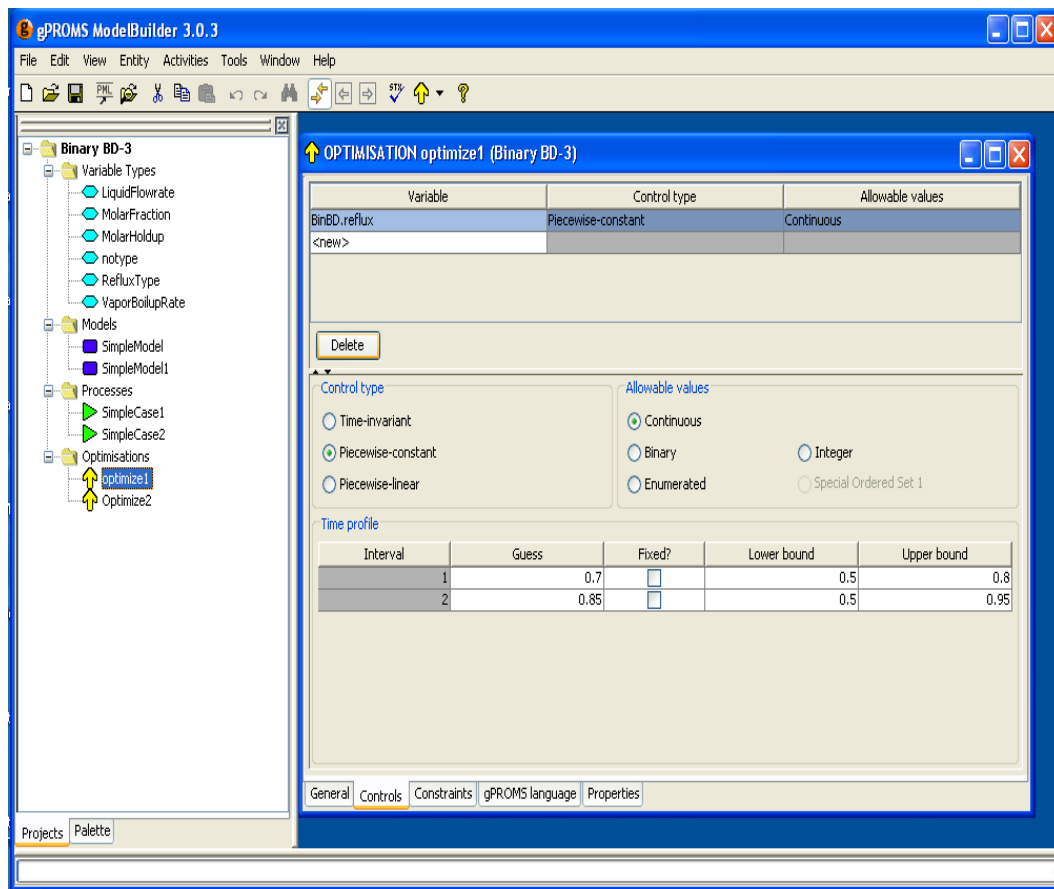
- General
- Controls
- Constraints

The control variables are divided into three constrains as follow:

- 1 Equality Constrains
- 2 In equality Constrains
- 3 Interior Point Constrains

The control variable profile are supported in the dynamic optimisation facilities in gPROMS, these are:

- Piecewise-constant controls.
- Piecewise-linear controls.



**Figure 3.3:** An Overview of the gPROMS (Part of the Optimisation File)

gPROMS provides built-in feature to plot different variable in MS Excel and designed to allow interacting dynamically with calculations performed in Microsoft Excel.

### **3.9 Conclusions**

Modelling and simulation of the *MultiVBD* column is discussed in this chapter. The optimisation problems are discussed briefly. Also the summary of the past work on optimisation of *MultiVBD* column has been highlighted. The optimisation problems are classified according to the characteristics of the objective function and control variable. This chapter includes brief general overview of the gPROMS modelling environment, some benefits and applications and features is presented and found to be easy, flexible and user-friendly software. Further information can be found at [www.psenterprise.com](http://www.psenterprise.com).

# CHAPTER 4

## PROCESS MODELS

### 4.1 Introduction

This chapter presents simple models for Conventional Batch Distillation (*CBD*) and Multivessel Batch Distillation (*MultiVBD*). The common assumptions based on which the models are developed are also listed.

### 4.2 Simple Model

The simple models used in this thesis are developed based on a number of assumptions for both configuration systems (Conventional and Multivessel batch distillation columns). These assumptions are introduced to simplify the model. These assumptions of constant relative volatility and equimolar overflow and include detailed plate-to-plate calculation. Further assumptions are listed below:

- a) Constant molar holdup for condenser and internal plates.
- b) Total condensation without sub-cooling.
- c) Negligible vapour holdup.
- d) Perfect mixing of liquid and vapour on all plates.
- e) Negligible heat losses.
- f) Negligible pressure drop across the column.

Robinson (1970); Mayur and Jackson (1971); Luyben (1988); Mujtaba and Macchietto (1992) used these assumptions for a simple model for simulation and optimisation of (CBD) column.

The model equations can be rearranged and solved; as a system of Ordinary Differential Equations (ODEs), or as a system of Differential and Algebraic Equations (DAEs).

The model is embedded in the *gPROMS* (general **P**rocess **M**odelling **S**ystem) software developed by Process System Enterprise Ltd. In most cases simple models are assumed to represent the actual process. In this thesis, two simple dynamic models are considered, one for conventional and the other one for multivessel batch distillation

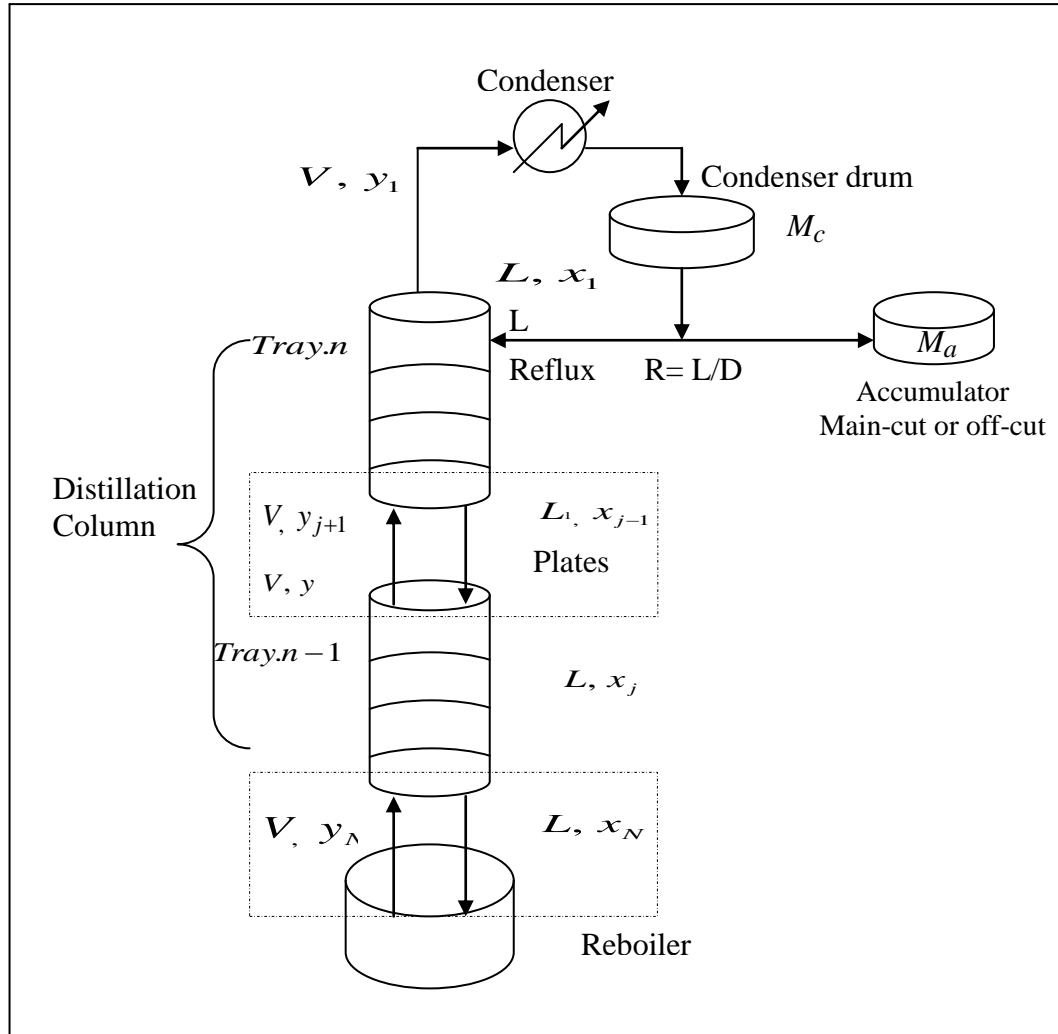
### **4.3 Simple Model for Conventional Batch Distillation (CBD)**

For conventional batch distillation column, the equations for the accumulator and condenser are presented and followed by equations for the plates in the column and the reboiler. The plates are counted from the top to the column.  $j$  refers to plates and  $i$  refers to components as shown in (Figure 1.4).

Condenser and accumulator,  $j = 1; i = 1$  to  $n_c$

The amount of product in the accumulator,  $Ma$  (Accumulator holdup) changes from time to time due to incoming liquid  $L_D$ , from the condenser according to the overall mass balance equations, where the entire condensate is initially returned to the column as reflux. After some time, a part of the overhead condensate is withdrawn continuously as distillate and it

is accumulated in the receivers as (products), and the other part is recycled into the column as reflux.



**Figure 4.1:** Conventional batch distillation column

Where:

$$\frac{dM_a}{dt} = L_D \quad (4.1)$$

The component mass balance in the accumulator is:

$$\frac{dx_{ai}}{dt} = \frac{L_D}{M_a} (x_{1i} - x_{ai}) \quad (4.2)$$

The holdup tank (condenser) contains an amount of liquid  $M_C$  which is kept constant at all time. The component balance for the holdup tank is:

$$\frac{dx_{1i}}{dt} = \frac{V}{M_c} (y_{2i} - x_{1i}) \quad (4.3)$$

The reflux ratio (internal) is defined as:

$$V = rL \quad (4.4)$$

where  $V$  is vapour flow,  $L$  is liquid flow and  $R$  is equal to

$$R = \frac{L}{V}$$

The distillate-rate to the accumulator or product tank is therefore:

$$L_D = V(1 - r) \quad (4.5)$$

Internal plates,  $j=2$  to  $(N-1)$ ;  $i = 1$  to  $n_c$

Like the condenser, the molar plate holdup (amount of liquid on the plates) remains at a constant value. The component balance on plate  $j$  is:

$$\frac{dx_{ji}}{dt} = \frac{V}{M_j} (y_{j+1,i} - y_{j,i}) + \frac{L}{M_j} (x_{j-1,i} - x_{j,i}) \quad (4.6)$$

The vapor liquid equilibrium relationship is written as:

$$y_{j,i} = \frac{\alpha_i x_{j,i}}{\sum_{k=1}^{n_c} \alpha_k x_{j,k}} \quad (4.7)$$

The reboiler,  $j = N$ ;  $i = 1$  to  $n_c$

The amount of mixture left in the reboiler depends on the liquid and the vapour flow rate through the column. The total mass balance is written as:

$$\frac{dM_N}{dt} = L - V \quad (4.8)$$

The component mass balance is:

$$M_N \frac{dx_{N,i}}{dt} = L(x_{N-1,i} - x_{N,i}) - V(y_N - x_{N,i}) \quad (4.9)$$

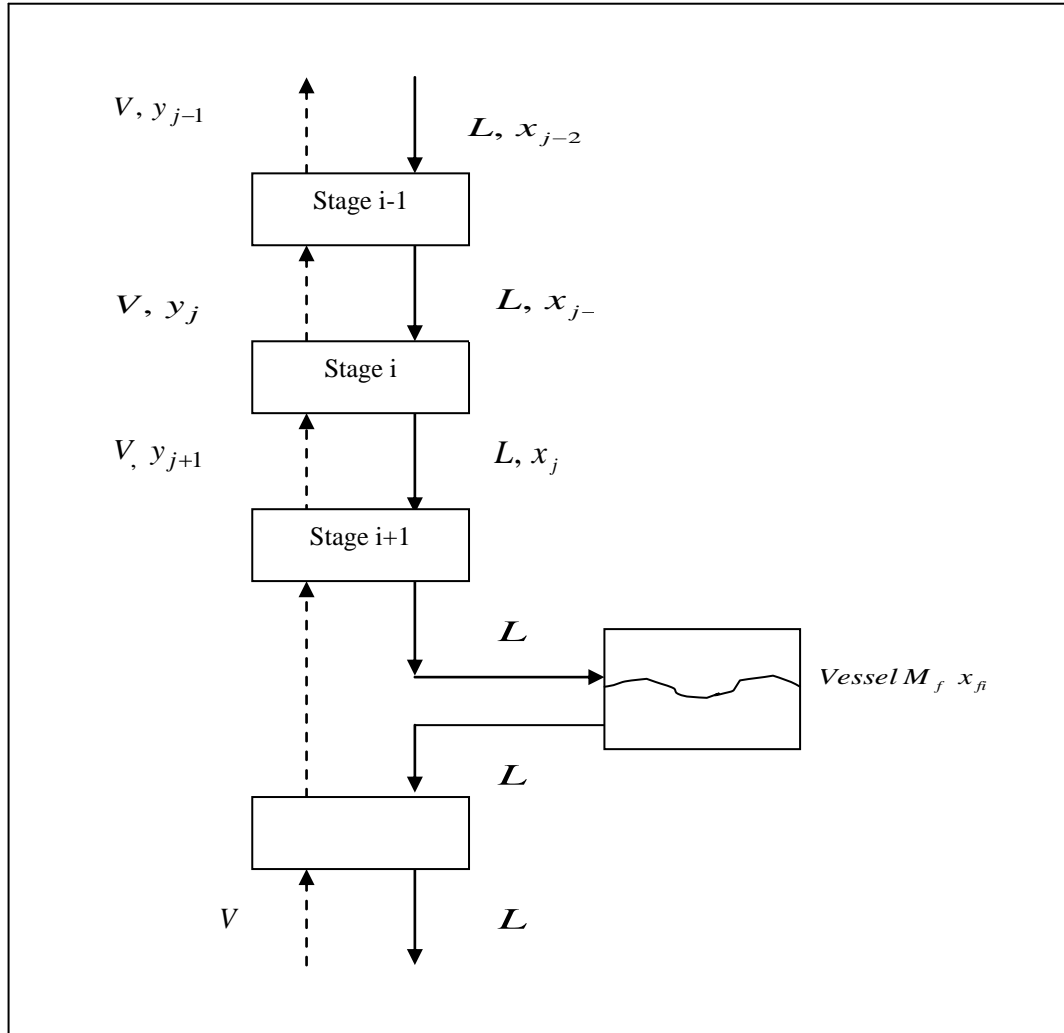
The vapour liquid equilibrium relationship is same as the equation (4.7) where  $j$  is replaced by  $N$ .

#### 4.4 Simple Model for Multivessel Batch Distillation Column

Referring to column configuration given in *Figure 2.7* in chapter 2 (P19), the tray model given in *Figure 4.2* where the distillation column is modeled as a stack of stages (counted from the top).

First, the equations for the condenser followed by equations for the plates in the column, intermediate vessels, and the reboiler are presented.

The plates are counted from the top to the column, where  $j$  refers to plates and  $i$  refer to components.



**Figure 4.2:** Connection of Plates and Vessel for (*MultiVBD*) Column

The total mass balance equation for the condenser is

$$\frac{dM_c}{dt} = V - L \quad (4.10)$$

The component mass balance in the condenser is

$$\frac{dx_{1i}}{dt} = \frac{V}{M_c} (y_{2i} - x_{1i}) \quad (4.11)$$

Internal plates,  $j=2$  to  $(N-1)$ ;  $i = 1$  to  $n_c$

The component mass balance on tray  $j$  is:

$$\frac{dx_{ji}}{dt} = \frac{V}{M_j} (y_{j+1,i} - y_{j,i}) + \frac{L}{M_j} (x_{j-1,i} - x_{j,i}) \quad (4.12)$$

The vapor liquid equilibrium relationship is:

for plates,  $j=2$  to  $(N-1)$ ; for component  $i = 1$  to  $n_c$

$$y_{j,i} = \frac{\alpha_i x_{j,i}}{\sum_{k=1}^{n_c} \alpha_k x_{j,k}} \quad (4.13)$$

Material balance for the intermediate vessels ( $i$ )

Total mass balance is written as

$$\frac{dM_{f_i}}{dt} = L_{f_{in}} - F_{out} \quad (4.14)$$

The component mass balance is

$$M_f \frac{dx_{f_i}}{dt} = L_{f_{in}} (x_{j_i} - x_{f_i}) \quad (4.15)$$

The other equations for the intermediate vessel (2) are the same as Equations (4.14 - 4.15) where  $Lf_{out}$  is replaced by  $Lf_{out-1}$ .

Material balance for the reboiler equations,  $j = N$ ;  $i = 1$  to  $n_c$

The total mass balance is written as:

$$\frac{dM_N}{dt} = L - V \quad (4.16)$$

The component mass balance is:

$$M_N \frac{dx_{N,i}}{dt} = L(x_{N-1,i} - x_{N,i}) - V(y_N - x_{N,i}) \quad (4.17)$$

The vapour liquid equilibrium relationship for reboiler is same as the equation (4.13) where  $j$  is replaced by  $N$ .

## 4.5 Conclusions

In this chapter, a simple dynamic model is considered for both configurations conventional (*CBD*) and unconventional (*MultiVBD*). This model is developed based on a number of assumptions and these assumptions are introduced to simplify the model and will be used in chapter 5, 6 and 7 using *gPROMS* software to solve the problems of binary and ternary separation processes. In this work, *gPROMS* modelling software is used for the modelling and dynamic optimisation of the batch distillation processes.

# CHAPTER 5

## OPTIMAL DESIGN AND OPERATION OF BINARY DISTILLATION

### 5.1 Introduction

Binary distillation is a separation of only two chemicals. A good example is separating ethanol alcohol (ethanol) from water. In the literature reviews and in the past work on the *MultiVBD* column, only multicomponent distillation is considered. No consideration was given to binary distillation and off-cut production for *MultiVBD* column. In this work, the *MultiVBD* column with binary distillation and with off-cut production is considered and discussed.

The operation of binary batch distillation is to separate a charge of specified quality and composition into a distillate (light component-main-cut), off and/or residue (heavy component), each with or without specified composition.

In this study, one scenario is considered. In this scenario a fixed batch time (in terms of fixed number of batches,  $N_B$ ), the optimal design (in terms of number of plates and vapour load) and operating policy (in terms of reflux ratio profile) are determined with strict product specifications.

Most recently, Low and Sorensen (2004) considered simultaneous design and operation optimisation for multipurpose batch distillation columns. Although  $V$  was used as an optimisation parameter, the results showed that in all cases  $V$  hit the upper bound. This was due to the fact that the profit could only be maximised with  $V$  hitting the upper bound leading to unlimited production of products. Also in their work, it was implicit that there is an unlimited market demand for the amount of products being produced. In reality, unplanned and unlimited production of products is not sustainable.

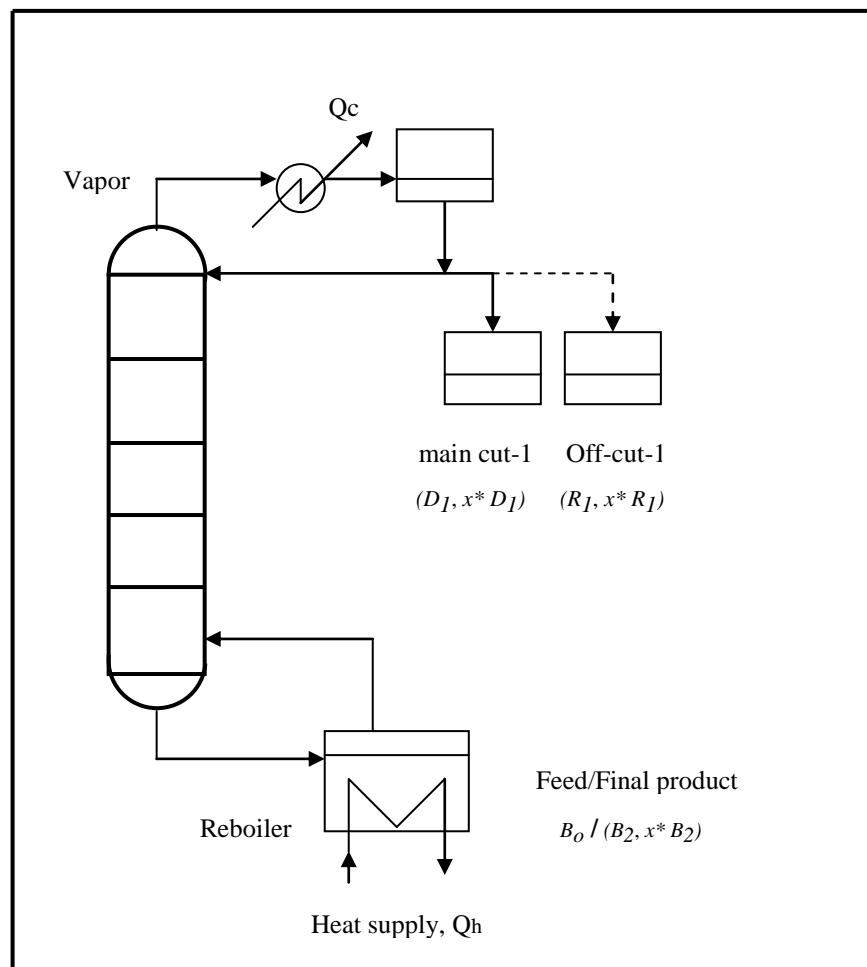
Low and Sorenson (2005) considered the optimal configuration, design and operation of batch distillation column with optimal vapour load  $V$  and number of trays  $N$  based on overall profitability for a given separation duty. However, strict product specification was not maintained and the vapour load hit the upper bound to minimise the batch time and to maximise the profit. This led to unlimited production of products based on the assumption that all products produced are saleable to maximise the profitability. In fact, the market demand  $N_B$  is more or less predictable a priori (at least for few years) within say  $\pm 10\%$

## **5.2 Operation Sequence**

The batch distillation operation can be schematically represented as a State Task Network (STN). A state (denoted by a circle) represents a specified material, and a task (rectangular box) represents the operational task (distillation) which transforms the input state(s) into the output state (Mujtaba and Macchietto, 1993).

For a binary distillation, a schematic of Conventional and Multivessel batch distillation columns are shown in *Figures 5.1, 5.2*.

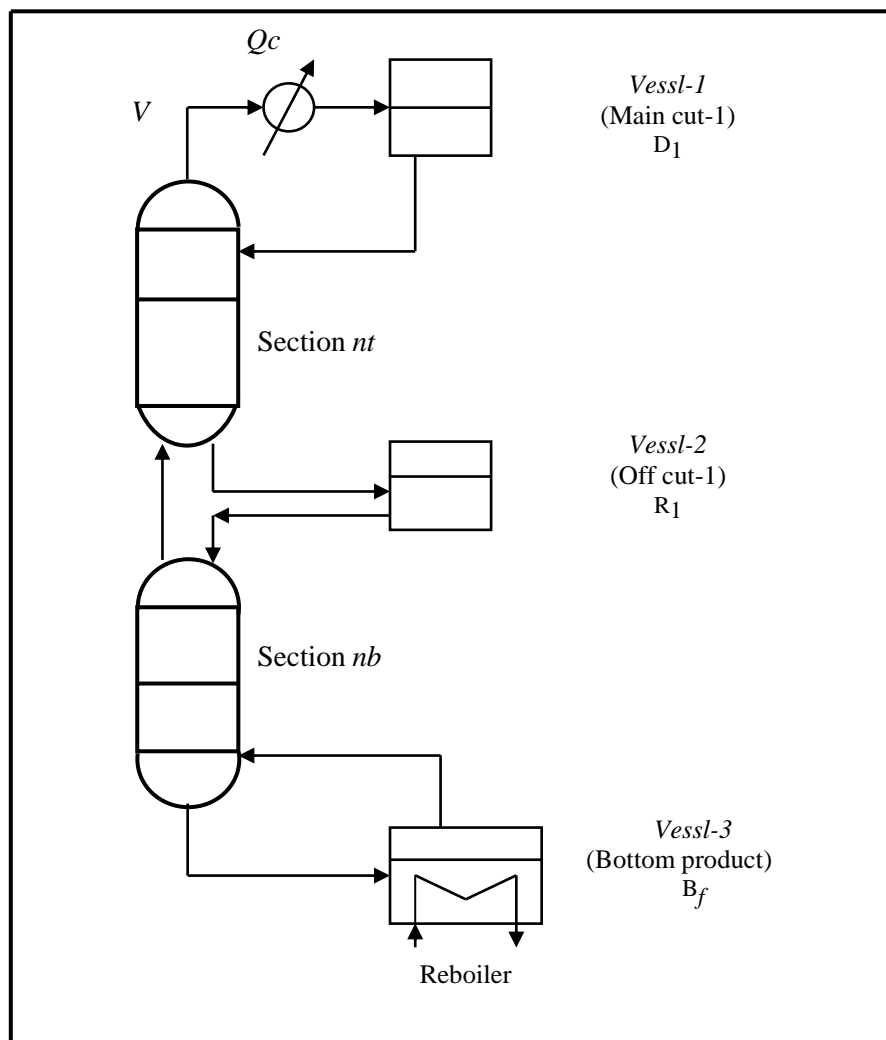
*Figure 5.3* shows the STN for this operation that is generated by joining sequentially a main-cut and an off-cut. The off-cut may be a valuable material and is usually stored for further separation or is recycled with the next batch. Its amount and composition are usually subject to optimisation. The bottom residual may or may not be a valuable material/product but may have to satisfy certain purity constraints due to environmental restrictions.



**Figure 5.1:** Conventional Batch Distillation Column (CBD)

For binary mixtures, there is usually one main-cut and one off-cut and there are only two basic production alternatives:

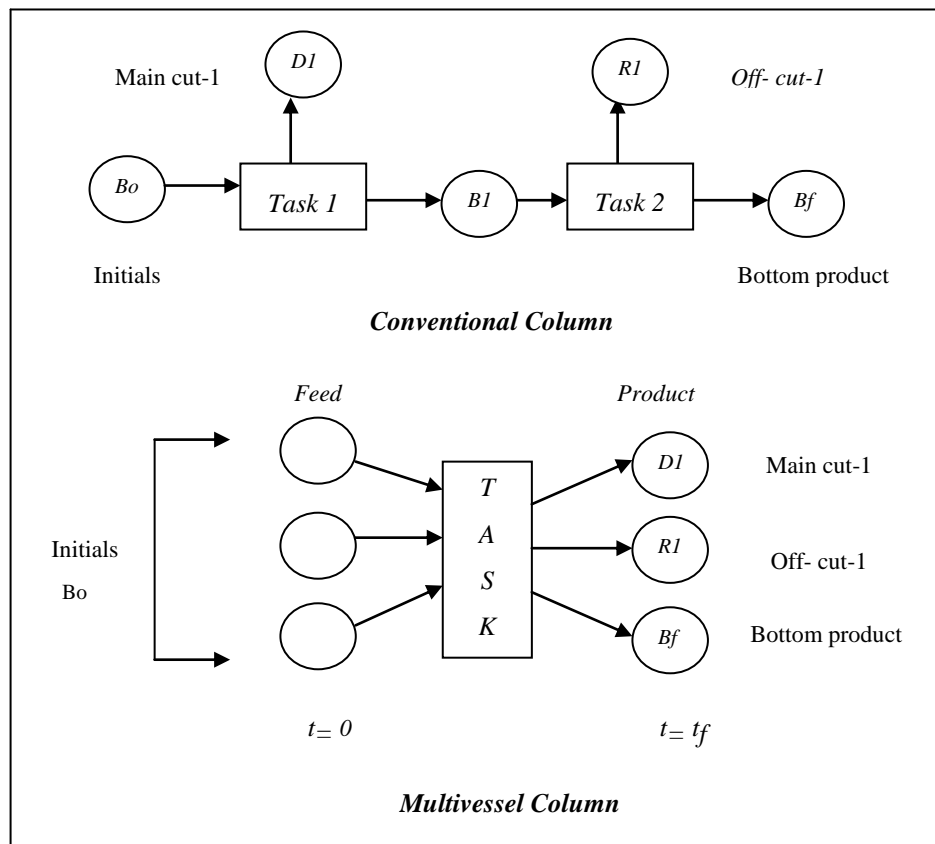
- i. A single main-cut is produced which must typically satisfy certain purity constraints. The bottom residue may also be a valuable product and/or may be required to satisfy certain purity constraints.
- ii. For such operation the *minimum time*, *maximum distillate* or *maximum profit* problems were discussed by Coward (1989); Kirkhof and Vissers (1978).



**Figure 5.2:** Multivessel Batch Distillation with Two Column Sections

- iii. A main-cut of specified purity is produced followed by an off-cut. The off-cut may be valuable material and is usually stored for further separation or is recycled with the next batch. Its amount and composition are usually subject to optimisation. The bottom residue may or may not be a valuable product but may have to satisfy certain purity constraint.

In the *MultiVBD* products will be produced simultaneously, while in conventional column *CBD* these will be produced sequentially as shown by State Task Network *STN* in (Figure 5.3), with one main-cut followed by an off-cut.



**Figure 5.3:** STN for Binary Batch Distillation

The significance of this schematic representation is to show clearly the number of products main-cut/off-cut to be produced. A state (denoted by a circle) represents a specified material, where  $B_o$  is raw material,  $D_I$  main product,  $R_I$  off-cut product and  $B_f$  is bottom product or residue, and a task (rectangular box) represents the operational task (distillation) which transforms the input state(s) into the output state(s) (Kondili *et al.*, 1988; Mujtaba and Macchietto, 1993). States are characterized by the amount and composition of the mixture residing in them. Tasks are characterized by operational attributes such as their duration, the reflux ratio profile used during the task, etc. Additional attributes of a distillation task are the set of values of all parameters (mainly operational) at the beginning and at the end of the task.

### 5.3 Optimisation Problem with Fixed Product Demand

The following design and operation optimisation for binary distillation is considered.

The optimisation problem can be defined as:

**Given** a binary feed mixture to be separated according to a predefined operation structure (*Figure 5.3*). The column configuration (*MultiVBD* or *CBD*), a set of product specifications (purities of key components in main products, amounts, etc.); production horizon ( $H$  hr/yr); product demand in terms of number of batches of product ( $N_B$ ).

**Optimise** Number of stages ( $N_S$  in different column sections for *MultiVBD* or  $N$  in *CBD* column, the vapour load ( $V$ ). In addition, the cut times ( $t_i$ ) and reflux ratio ( $r$ ) in each cut of Conventional column.

**Maximise** The total profit ( $P$ )

**Subject to** Any constraints (model equations, bounds on the variables, etc.).

Mathematically, the problem ( $OP$ ) can be written as:

$$\begin{array}{ll}
 \mathbf{OP} \text{ (objective)} & \begin{array}{l} \mathbf{Max} \\ N_S \text{ (or } N), V \text{ (and } r_i, t_i) \end{array} & \mathbf{P} \\
 \\
 \text{Subject to:} & \begin{array}{l} \text{Process Model Equations} \\ \text{Fixed product demands} \\ \text{Product specifications} \\ \text{Bounds on } N_S \text{ (or } N), V, \text{ (and } r_i, t_i) \\ \text{Fixed batch time} \end{array} & \begin{array}{l} \text{(Equality constraint)} \\ \text{(Equality constraint)} \\ \text{(Equality constraint)} \\ \text{(Inequality constraint)} \\ \text{(Equality constraint)} \end{array}
 \end{array}$$

The objective function is profit per year ((\$/year) Mujtaba (2004) can be calculated using:

$$\begin{aligned}
 \text{Profit (\$/year)} = P = & (\text{product revenues} - \text{raw material cost} - \text{operating cost}) \text{ batch} \times \\
 & \times \text{number of batches per year} - \text{annualised capital cost}
 \end{aligned}$$

$$P = (C_1 D_1 + C_2 R_1 - C_3 B_0 - OC_b) \times N_B - ACC \quad (5.1)$$

Where,  $C_1$ ,  $C_2$ , and  $C_3$  are the prices of main-cut, off-cut, and raw material cost respectively.

$$N_B = \text{Number of Batches / Year} = H / (t_b + t_s) \quad (5.2)$$

$$(C_1 D_1) = \text{Product revenue (\$/batch)}$$

$$OC_b = \text{Operating cost (\$/batch)} = (K_3 V / A) \times (t_b - t_s) \quad (5.3)$$

( $OC$ , Guthrie's correlations)

$$ACC = \text{Annualised capital cost (\$/yr), } K_1 V^{0.5} N^{0.8} + K_2 V^{0.65} \quad (5.4)$$

$V$  = Vapour load (kmol/hr)

$A$  = Dimensionless constant for (OC) operating cost (8000)

$H$  = Production horizon = 8000 h/year

$K_1$  = Constant for annualised capital costs equation (1500)

$K_2$  = Constant for annualised capital costs equation (9500)

$K_3$  = Utility costs coefficient constant for operating cost equation (180)

$t_b$  = Batch time (hr),  $t_s$  = Set-up time (constant) = 0.5 hr

Note, Furlonge *et al.* (1999) reported that variable hold-ups in the vessels of *MultiVBD* reduce energy consumption. In this work, we distributed the feed in different vessels according to the product profiles calculated a priori. Also, the reflux ratio for conventional column is divided into two time intervals for task 1 to produce (main-cut) and one time interval for task 2 to produce (off-cut). Thus a total of 3 reflux ratio levels and 3 switching times are optimised for the whole multiperiod operation.

The above optimisation problem is solved using *gPROMS* optimiser. The dynamic optimisation problem is converted to nonlinear programming problem by Control Vector Parameterisation (*CVP*) technique and is solved using efficient *SQP* method. There are two standard mathematical solvers available in *gPROMS* for solving dynamic optimisation problems. Both are based on a (*CVP*) approach which assumes that the time varying control interval are piecewise constant or piecewise linear functions of time over a specified number of control intervals.

## 5.4 Example Problems

In this chapter, a binary distillation is considered and simple process models are developed in *gPROMS* for both configurations and the optimisation problems are solved using the built-in facilities within *gPROMS*.

The input data for this problem is presented in (*Table 5.1*). The molar quantity of initial charge is same for both configurations (10 kmol per batch of the feed). For simplicity, the amount of *product A* (main-cut-1) to be produced is 1.99 kmol/batch with 95% purity molefraction, so the total amount of this product will be 2915.75 kmol/yr with number of batches are 1465.20 batch/year is to be produced from 14652 kmol/yr of total feed of a binary mixture (*A* and *B*). Due to high purity requirement of *product B*, intermediate off-cut needs to be produced with no more than 40% purity in terms of component *A*.

Component *B* is not a valuable product but fixed at 95% molefraction for disposal meeting the environmental restriction. The value of the off-cut by product and the final bottom residue are negligible. The reflux ratio control is discretised into two intervals for step 1 and one interval during step 2 for *CBD* column.

*MultiVBD* column has 3 vessels including the reboiler and condenser holdup tank (2 column sections). Both *CBD* and *MultiVBD* columns are available for period of 8000 hrs/yr. The set up time for each batch of operation is 30 minutes. The total number of batches will therefore be 1465.20 per year and the individual batch time would be 4.96 hr, all productions are achieved on specification.

Three different cases are considered, corresponding to the optimisation of vapour load and number of stages to maximise the profit. Based on the feed and product specifications, the overall mass balance and component balance (using equations 5.5 - 5.10) will give  $D =$  Total Distillate Product = 1.99 kmol (per batch),  $R =$  Total off-cut Product = 2.03 kmol (per batch) and  $B =$  Total Bottom Product = 5.98 kmol (per batch).

$$B_0 = D_1 + R_1 + B_1 \quad (5.5)$$

$$B_0 x_{B0} = D_1 x_{D1} + R_1 x_{R1} + B_1 x_{B1} \quad (5.6)$$

$$\sum x_{B0} = 1 \quad (5.7)$$

$$\sum x_{D1} = 1 \quad (5.8)$$

$$\sum x_{R1} = 1 \quad (5.9)$$

$$\sum x_{B1} = 1 \quad (5.10)$$

Given:  $B_0 = 10$  kmol,  $x_{1B0} = 0.30$ ,  $x_{2B0} = 0.70$

Product specifications:  $x_{1D1} = 0.95$ ,  $x_{1R1} = 0.40$ , and  $x_{2B1} = 0.95$

Let;  $C_1 =$  Top product price (main-cut) = \$20/kmol.

$C_2 =$  Intermediate price product (off-cut) = \$0.0/kmol (not a desired product).

$C_3 =$  Raw material cost (feed) = \$1.0/kmol.

With reference to two scenarios as shown in *Figure 5.3*, the typical design parameters would be the number of stages  $N$  and vapour load  $V$  and typical operating parameters would be reflux ratio for *CBD* column with fixed batch time  $t_b$ .

The investigations are carried out in the following sequence:

- Effect of the number of stages on batch distillation for a given vapour load.
- Effect of the vapour load on batch distillation for a given number of stages.
- Optimum design and operation of binary distillation for *CBD* and *MultiVBD*

In this chapter, we considered:

- Both designs of (number of stages and vapour load) are optimised.
- Fixed product demand scenario.
- The off-cut ( $R_1$ ) is not a desired product.

**Table 5.1:** Input Data for Binary Distillation of *CBD* and *MultiVBD* Columns

Total Fresh Feed, $B_0$ , kmol	= 10
Feed Composition, $x_{B_0}$ , mole fraction	= <0.3, 0.7>
<u>Column Holdup, kmol:</u>	
Condenser	= 0.1
Internal Plates	= 0.025
Number of Components	= 2
Relative Volatility, $\alpha$	= <3.0, 1.0>
Purity of Main-cut-1, $x_{1D1}$ , mol fraction	= 0.95
Composition of Off-cut-1, $x_{1R1}$ , mol fraction	= 0.40
Composition of Bottom Residue, $x_{2B1}$ , mol fraction	= 0.95
Number of batches, yr	= 1465.2

### 5.4.1 Effect of Number of Stages

A binary distillations is considered for *MultiVBD* and *CBD* columns to study the effect of number of stage on the operating cost (*OC*), annual capital cost (*ACC*) and annual profit.

The study was made using  $V = 3$  kmol/hr and the number of stages are optimised to maximise a profit function. The input data for this problem are given in *Table 5.1*.

The product demand and quality (purity) of main-cut and off-cut are achieved to the given specifications.

In this investigation vapour load  $V$  is fixed and the number of stages  $N$  is varied for both columns, the operating time is fixed in terms of (number of batches). The optimisation problem will now have to determine the optimum values of  $N$  for a given  $V = 3$  kmol/hr therefore, the maximum profit could be achieved with optimum  $N$ . For each number of stages, the results in terms of operating cost (*OC*), annual capital cost (*ACC*), reflux ratio ( $r$ ) for *CBD* column, and achievable profits ( $P$ ) are summarised in *Table 5.2*

The reflux ratio ( $r$ ) is discretised into two time intervals for task 1 (two reflux ratio for the main-cut) and one time interval for task 2 (one reflux ration for the off-cut). Thus a total of 3 reflux ratio levels and 3 switching times are optimised for the whole multiperiod operation.

**Table 5.2:** Summary of the Results – (Effect of  $N$ ) with Fixed  $V = 3$ 

	$N$	$D_1$	$t_1$	$R_1$	$t_2$	$OC$	$ACC$	$P$	$P$
<b>Configuration</b>		kmol	hr	kmol	hr	\$/b	\$/yr	\$/b	\$/yr
<i>CBD</i>	6	1.99	3.43	2.03	1.53	0.368	30296	8.75	12827.0
<i>MultiVBD</i>	5 (3, 2)	1.99	4.96	2.03	–	0.368	28817	9.76	<b>14305.6</b>
Reflux Ratio Profile for <i>CBD</i> :									
		Main-Cut 1 ( $D_1$ )			Off-Cut ( $R_1$ )				
Reflux ratio (r)		0.779			0.833			0.557	
Switching Time (hr)		0.0 - 1.67			1.67 - 3.43			4.96	

### 5.4.1.1 Results

In *Table 5.2*, under fixed product demand in terms of number of batches ( $N_B$ ), the  $N_B$  is fixed with 1465.20 (batch/ year) to produce a total distillate product of main-cut 2915.8 kmol/year for both configurations based on the feed and product specifications, the optimum number of stages ( $N$ ) for *MultiVBD* column is 5 stages (3 stages at the top of column section, and 2 stages at the bottom of column section), that will give the maximum profit ( $P$ ) of 14305.6 \$/yr, while the optimum number of stages ( $N$ ) for *CBD* is 6 columns with the optimal reflux profiles in task 1 ( main-cut) are 0.779 and 0.833 and in task 2 (off-cut) is 0.557 to ensure that the very high purity for requirements of component 1 and off-cut, that will give the maximum profit ( $P$ ) of 12827.0 \$/yr.

The maximum profit of *MultiVBD* column in this case is about 10.4% more compared to the *CBD* column due to lower number of stages which is required to achieve the product specification. A higher  $N$  and  $V$  will always increase the capital cost and operating cost and this will reduce the total profit.

## 5.4.2 Effect of Vapour load

A binary distillations is considered for *MultiVBD* and *CBD* columns to study the effect of vapour load on the operating cost (*OC*), annual capital cost (*ACC*) and total profit. The study was made using  $N = 8$  and the vapour load is optimised to maximise a profit function.

In this investigation, number of stages  $N$  is fixed and vapour load  $V$  is varied for both column with fixed operating time in terms of (number of batches). The optimisation problem will now have to determine the optimum values of  $V$  for a given number of stages  $N = 8$ , therefore, the maximum profit could be achieved with optimum  $V$ .

**Table 5.3:** Summary of the Results – (Effect of  $V$ ) with Fixed  $N = 8$

	$V$	$D_1$	$t_1$	$R_1$	$t_2$	$OC$	$ACC$	$P$	$P$
<b>Configuration</b>	Kmol/hr	kmol	hr	kmol	hr	\$/b	\$/yr	\$/b	\$/yr
<i>CBD</i>	2.53	1.99	3.43	2.03	1.53	0.311	29961	9.04	13246.7
<i>MultiVBD</i>	1.96	1.99	4.96	2.03	–	0.240	24797	11.95	<b>17513.7</b>

Reflux Ratio Profile for <i>CBD</i> :			
	Main-Cut 1 ( $D_1$ )		Off-Cut ( $R_1$ )
Reflux ratio	0.689		0.478
Switching Time (hr)	0.0 - 1.67		1.67 - 3.43

### 5.4.2.1 Results

For each vapour load, the results in terms of operating cost (*OC*), annual capital cost (*ACC*), reflux ratio ( $r$ ) for *CBD* column and achievable profits ( $P$ ) are summarised in *Table 5.3*. The reflux ratio ( $r$ ) is discretised into two time intervals for task 1 and one time interval

for task 2. Thus a total of 3 reflux ratio levels and 3 switching times are optimised for the whole multiperiod operation.

Also in *Table 5.3*, under fixed product demand in terms of number of batches  $N_B = 1465.20$  per year and strict product specification, the optimum vapour load for *CBD* column is 2.53 kmol/hr with the optimal reflux profiles in task 1 (main-cut) are 0.689 and 0.848 and in task 2 (off-cut) is 0.478 to ensure that the very high purity for requirements of component 1 and off-cut, that will give the maximum profit ( $P$ ) of 13246.7 \$/yr, while in *MultiVBD* column the optimal vapour load is 1.96 kmol/hr, that will give the maximum profit ( $P$ ) of 17513.7 \$/yr. These results clearly show that decreasing vapour load  $V$  will decrease the capital cost and increase the profit.

Again, the profitability of *MultiVBD* column is 24.4% more compared to *CBD* column due to low vapour load required to achieve the desired specifications. The operating cost (an indirect measure of the energy cost and environmental impact) is more than 22.3% lower of *MultiVBD* system.

### 5.4.3 Simultaneous Optimisation of $N$ and $V$

Here we consider simultaneous optimisation of design (number of plates  $N$  and vapour load  $V$ ) and operation (reflux ratio  $r$ , operating time  $t$ ) with fixed product demands and fixed separation sequence as shown in *Figure 5.3*.

The optimization problem will have to determine the optimal values of  $N$  and  $V$ , for given  $t_b = 4.96\text{h}$  and  $D_1 = 1.99$  kmol/batch, which will maximize the annual profit. For the sake of

clear discussion and to show that there is only one optimum combination of  $N$  and  $V$  for given product demand and product specification.

The comparison between ( $CBD$  and  $MultiVBD$ ) is summarised in *Table 5.4* in terms of operating cost, annual capital and achievable profits for both configurations.

**Table 5.4:** Maximum Profit – (Optimum  $V$  and  $N$ )

	$V$	$N$	$D_1$	$t_1$	$R_1$	$t_2$	$OC$	$ACC$	$P$	$P$
<b>Configuration</b>	Kmol/hr		Kmol/b	hr	Kmol/b	hr	\$/b	\$/yr	\$/b	\$/yr
<i>CBD</i>	<b>2.70</b>	<b>7</b>	1.99	3.43	2.03	1.53	0.331	29809	9.12	13368.1
<i>MultiVBD</i>	<b>2.05</b>	<b>7</b> (5, 2)	1.99	4.96	2.03	–	0.252	25335	12.26	<b>17959.0</b>

Reflux Ratio Profile for CBD:

	Main-Cut 1 ( $D_1$ )		Off-Cut ( $R_1$ )
Reflux ratio	0.701	0.852	0.510
Switching Time (hr)	0.0 - 1.67	1.67 - 3.43	4.96

### 5.4.3.1 Results

From *Table 5.4* the optimum  $V$  and  $N$  for both column configurations are considered, where optimal vapour load for ( $MultiVBD$ ) column  $V = 2.05$  kmol with optimal number of stages  $N = 7$  stages (5 stages at the top of column section and 2 stages at the bottom of column section), while for  $CBD$  column the optimal vapour load  $V = 2.70$  kmol and optimal number of stages  $N = 7$  stages with the optimal reflux ratio 0.701 and 0.852 for main-cut 1 and 0.510 for off-cut 1.

Figure 5.4 shows the distillate products (composition vs time) for case-3, where the desired specification of the products (main-cut,  $D_1$ ) and (off-cut,  $R_1$ ) are achieved and meet the product specifications (0.95 and 0.05) respectively.

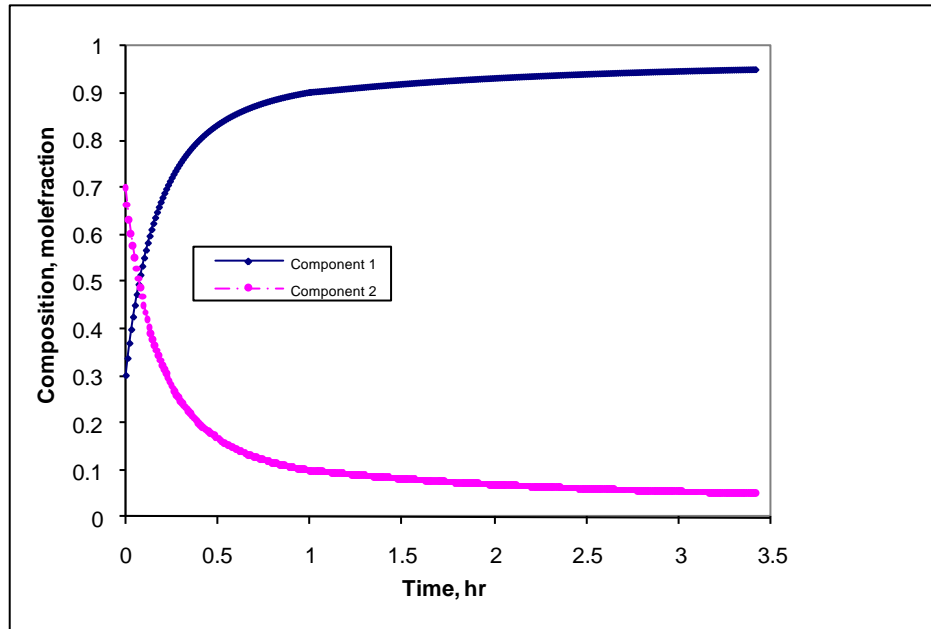


Figure 5.4: Composition of main-cut and off-cut for *MultiVBD* (Case-3)

The results also show the operating cost per batch, annualised capital cost, profit per batch and per year. The vapour load for the *MultiVBD* column is about 24.1% lower compared to *CBD* column and the operating cost is 23.9% lower. Finally, the overall profit realised by *MultiVBD* column is about 25.6% more than by *CBD* column.

Three different cases are considered, corresponding to the optimisation of ( $V$  and  $N$ ) and operation of reflux ratio for *CBD* column, where the operating time is fixed in terms of (No. of batches) and the off-cut ( $R_1$ ) is not a desired product.

The investigations are carried out in the following sequence:

- Effect of number of stages ( $N$ ) on batch distillation for a given vapour load.
- Effect of vapour load ( $V$ ) on batch distillation for a given number of stages.
- Optimum design ( $N, V$ ) and operation of binary distillation for *CBD* and *MultiVBD*.

**Table 5.5:** Summary of the optimisation for different processes (Maximum Profit)

Configuration	Optimisation	Vapour load $V$	Number of Plates $N$	$N_B$ $yr$	$DI$ $Kmol/yr$	$P$ $\$/yr$	Profitability %
<i>CBD</i>	N	3	6	1465.20	2915.8	12827.0	
<i>MultiVBD</i>	N	3	5 (3,2)	1465.20	2915.8	<b>14305.6</b>	<b>10.4</b> more
<i>CBD</i>	V	2.53	8	1465.20	2915.8	13246.7	
<i>MultiVBD</i>	V	1.96	8 (5,3)	1465.20	2915.8	<b>17513.7</b>	<b>24.4</b> more
<i>CBD</i>	$N \& V$	7	2.70	1465.20	2915.8	13246.7	
<i>MultiVBD</i>	$N \& V$	7 (5, 2)	2.05	1465.20	2915.8	<b>13368.1</b>	<b>25.6</b> more

The profitability in *Tables 5.2, 5.3* and *5.4* are summarised in *Table 5.5*. The product demand for both configurations is fixed in terms of number of batches ( $N_B=1465.20/yr$ ) where, the number of stages is optimised for a given vapour load in case-1. The vapour load is optimised for a given number of stages in case-2 and in case-3 both vapour load and number of stages are optimise to achieve optimum profit for all cases. From *Table 5.5*, the results of *MultiVBD* column were found to be more profitable than *CBD* column this is due to low vapour load ( $V$ ) which is required to achieve the desired specifications.

## 5.5 Conclusions

In this work the optimum design and operation of binary separation under fixed product demand in terms of fixed number of batches is presented for *CBD* and *MultiVBD* columns.

For the first time, fixed product demand scenario has been built-in in the optimisation problem formulation leading to a different optimisation problem formulation compared to that required under the unlimited product demand scenario. For unlimited market demand, the vapour load and number of stages could be unlimited and will always favour the highest possible value to maximise the profit.

Finally, the results presented in *Tables 5.5* clearly show that the *MultiVBD* column was found to be significantly more profitable than in *CBD* column and demonstrated a reduction in energy consumption and the economical benefit becomes more apparent.

# CHAPTER 6

## MULTICOMPONENT MULTIVESSL BATCH

### DISTILLATION COLUMN – STN 1

#### 6.1 Introduction

The batch distillation operation can be schematically represented as a State Task Network (*STN*). A state (denoted by a circle) represents a specified material, and a task (rectangular box) represents the operational task (distillation) which transforms the input state(s) into the output state(s) (Mujtaba and Macchietto, 1993). For example, *Figure 6.1* shows distillation task producing a main-cut 1 (*D1*), off-cut 1 (*R1*), main-cut 2 (*D2*), and a bottom residue product (*Bf*) from an initial charge (*Bo*). States are characterised by the amount and composition of the mixture residing in them. Tasks are characterised by operational attributes such as their duration, the reflux ratio profile used during the task, etc. This operation task is presented only for conventional batch distillation column by (Mujtaba and Macchietto, 1993). This thesis will represent with Multivessel batch distillation column for the first time as shown in *Figure 6.1*.

Part of this chapter is published in: M.T. Mahmud, I.M.Mujtaba and M Emtir, “Optimal design and operation of Multivessel batch distillation column with fixed product demand and strict product specifications” *Comp Aided Chemical Eng., Vol 25, ESCAPE, 2008*

The case study in this chapter is for ternary distillation to maximise a general profit function ( $P$ ) with respect to the net production, specifications, and profitability using a *MultiVBD* and compared to a *CBD* column used by Mujtaba and Macchietto (1993).

The operation of ternary mixture is to separate a charge of specified quantity and composition into a distillate ((light component), off and/or main-cuts, (middle component) and residue (heavy component), each with or without specified composition.

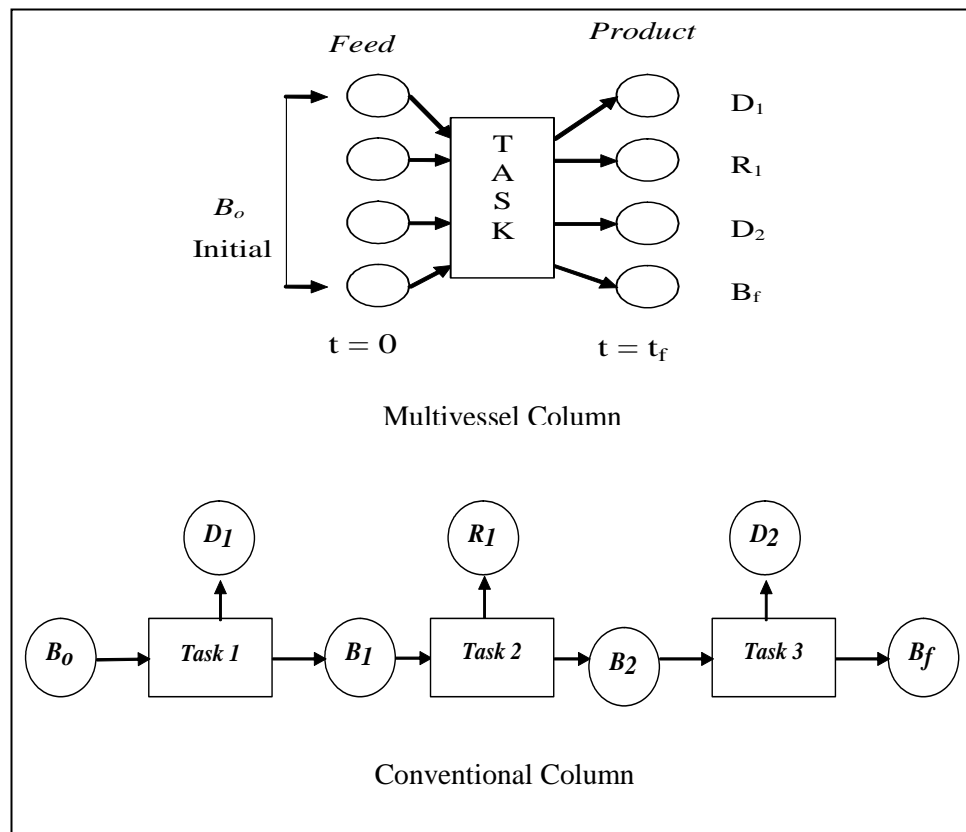
Off-cut production and recycling played an important role in efficient separation of binary and multicomponent mixtures using batch distillation. However, the research in this area is handful and all the investigations were concerned with only operating optimisation in terms of minimisation of batch time or maximisation of productivity (amount of main products per unit time).

Mujtaba and Macchietto (1993) considered the profit calculation with fixed operation cost (fixed design) in terms of number of plates and vapor flow rate, and exclude set-up time and capital cost. However, the optimization of their study was not geared for fixed product demand scenario. That leads to unlimited production of products and their profitability calculations were based on the assumption that all products produced are saleable (open market). Also, there were no penalties for over or under production, production of off-cuts and customer dissatisfaction.

Mujtaba and Macchietto (1996) proposed a method for *CBD* column to determine optimal design (number of plates) and operation for multicomponent batch distillation of a given feed mixture with fixed *STN* operation that with each main cut followed by an off-cut

(Figure 6.1), with fixed vapor flow rate and based on a rigorous optimisation with a detailed but constant molar holdup. They proposed a two loop optimisation framework, in the outer loop the profit is maximised, while optimising the number of plates, amount off-cuts and compositions of the off-cut. In the inner loop the batch time is minimised for each cut, while optimising the reflux ratio for the cut to satisfy the product purities. The method was demonstrated using a ternary separation. However, the optimisation study of Mujtaba and Macchietto (1996) was not geared for fixed product demand scenario.

In this chapter, the *STN* (Figure 6.1) for *MultiVBD* and *CBD* is considered with two main cuts and one off-cut in between to achieve maximum overall profit with the fixed amount of product and the desired purity separation.



**Figure 6.1:** *STN* for Multivessel and Conventional Column with Two Main-Cuts

## 6.2 Case Study and Comparison of *MultiVBD* with *CBD*

The case study in this chapter is based on *Case-1* study of Mujtaba and Macchietto (1993) where a *CBD* column was used. In the *CBD*, the feed is charged wholly into the reboiler also piecewise constant reflux ratios with two intervals were used for each cut. In the *MultiVBD*, the feed is distributed among the reboiler, two side vessels in between, and reflux drum as Furlonge *et al.* (1999). All the holdups are kept constant throughout the operation, which takes place under total reflux to achieve the desired specifications.

It was the first attempt to solve the problem with *MultiVBD*. To simplify the comparison, the model specification, product pricing, and setup time are similar to those of the *Case-1* study as (base case) given in *Table 6.1*.

### 6.2.1 Product Demand and Specifications

A total of 2555 kmol/yr of *Product A* with 95% purity (mole fraction) and 1214 kmol/yr of *Product B* with 95% purity (mole fraction) are to be produced from 9791.90 kmol/yr of a ternary mixture (*A*, *B*, and *C*) with feed composition of  $\langle 0.30, 0.20, 0.50 \rangle$  molefraction and relative volatility  $\alpha = \langle 8.0, 4.0, 1.0 \rangle$ . Due to high purity demand of *Product B*, an intermediate off-cut is needed to be produced with no more than 60% purity in component *A*. Component *C* is not a valuable product.

The maximum capacity of the *MultiVBD* column is 10kmol/batch and has 4 vessels including the reboiler, condenser, and two holdup tanks with (3 column sections). Both *CBD* and the *MultiVBD* columns are available for a period of 8000 hrs/yr. The set up time

for each batch of operation is 30 minutes. The total number of batches will therefore be 979.19 per year and the individual batch time would be 7.67 hr. The input data for this problem are given in *Table 6.1*.

**Table 6.1:** Input Data for Ternary Distillation of *CBD* and *MultiVBD* Columns

Total Fresh Feed, $B_0$ , kmol	= 10
Feed Composition, $x_{B_0}$ , mole fraction	= <0.3, 0.2, 0.5>
<u>Column Holdup, kmol:</u>	
Condenser	= 0.1
Internal Plates	= 0.0125
Number of Components	= 3
Number of Batches, yr	= 979.19
Relative Volatility, $\alpha$	= <8.0, 4.0, 1.0>
Purity of Main-cut-1, $x^1_{D_1}$ , mol fraction	= 0.95
Composition of Off-cut-1, $x^1_{R_1}$ , mol fraction	= 0.60
Purity of Main-cut-2, $x^2_{D_2}$ , mol fraction	= 0.95
Total Batch Processing Time, hr	= 7.67
Feed cost, (\$/kmol)	= 1.0
Product Price, (\$/kmol)	= 20.0

For a batch with 10 kmol feed mixture ( $B_0$ ), the product profiles for both configurations with desired number of batches are given in *Table 6.2*, these profiles are calculated using steady state mass balance (Miladi and Mujtaba, 2006) as: *Product A* = 2.61 kmol/batch ( $D_1$ ); *Product B* = 1.24 kmol/batch ( $D_2$ ); Intermediate Off-Cut = 0.83 kmol/batch ( $R_1$ ) and

Bottom Residue (in the reboiler) = 5.32 kmol/batch ( $B_f$ ). The simple dynamic column model was used for this example. In *MultiVBD* column, the products will be produced simultaneously while in the conventional column these will be produced sequentially as shown by State Task Network *STN* in *Figure 6.1*. In this specific operation the bottom residue product ( $B_f, x_{B_3}$ ) was not a desired product, and may be valuable product but may have to satisfy certain purity constraint.

The optimisation problem is solved using *gPROMS* software. Note, for *CBD* column, two reflux intervals were considered for each cut and the reflux ratio in each interval was assumed to be piecewise constant (Mujtaba, 2004).

## 6.2.2 Objective Function and Optimisation Problem Formulation

In this case, two different profit functions (hourly and annually) are used for both column configurations. The first profit function can be as general as desired (Mujtaba and Macchietto, 1993) to reflect both annulised investment (e.g. column, reboiler, condenser, etc) and operating cost (e.g. steam), and defined as:

$$Profit (\$/hr) = P = \frac{C_{D1}D_1 + C_{D2}D_2 + C_{B3}B_3 + C_{R1}R_1 - C_{B0}B_o}{t_1 + t_2 + t_3} \quad (6.1)$$

Where;  $C_{D1}$ ,  $C_{D2}$ ,  $C_{B3}$ , and  $C_{R1}$  are the prices (\$/kmol) of the main-cuts, bottom and off-cut-1 product.

$C_{B0}$  is the cost (\$/kmol) of the fresh feed mixture and  $C_{fc}$  is operating cost = 5.0 \$/hr,

$C_{fc}$  is fixed design (in terms of number of plates and vapour flow rate).

The values of the off-cut product and final residue are to be zero

where,  $C_{B3} = C_{R1} = 0.0$ .

The production times for tasks 1, 2, and 3 is  $t_1 t_2 t_3$ , respectively and is equal to (7.67hrs)

and the amounts of the products are  $D_1, R_1, D_2, B_3$

The second profit function (Miladi and Mujtaba, 2004) as shown in chapter 5 Eq. (5.1) and also the optimisation problems are presented in *Chapter 5*.

### 6.2.3 Results and Discussions

Using the first profit function of Mujtaba and Macchietto (1993) the results of *Table 6.3* show the total profit for both configurations = 28,053.9 \$/year due to fixed operating cost =5.0 \$/hr in terms of number of stages and vapour flow rate which is to produce total amount of  $D_1 = 2555.4$ ,  $D_2 = 1214.0$ ,  $B_3 = 5208.8$  and  $R_1 = 821.6$  kmol/year, respectively, and the number of batches is 979.19 per year, with total charge of feed is 9791.90 kmol/year, and with total time of 8000.0 hr a year.

*Table 6.2* summarised the product profiles for both configurations with desired number of batches, total charge of the feed and the amount of required products in each batch. For instance, 1 batch of 10 kmol feed will produce 2.6 kmol of  $D_1$ , 0.83 kmol of  $R_1$ , 1.24 kmol of  $D_2$ , and 5.23 kmol of  $B_f$  and will require a batch time of 8.17 hr This will make a profit of \$28.7. With 979.19 batches a year (8000 hrs) and 9791.90 kmol of feed, the total product

of main-cut  $D_1$  is 2555.4 kmol, the total product of off-cut  $R_1$  is 821.6 kmol, the total product of main-cut  $D_2$  is 1214.0 kmol and the total product of bottom residue  $B_f$  is 5208.0 kmol. This will make a total profit of 28,053.8 in a year.

**Table 6.2:** Profit Profiles for *CBD* and *MultiVBD* Columns with Desired  $N_B$

<b>No. of batches</b> $N_B$	$D_1$ kmol/yr	$R_1$ Kmol/yr	$D_2$ Kmol/yr	$B_f$ Kmol/yr	<i>Total charge</i> Kmol/yr	<i>Total profit</i> \$/batch	<i>Total time</i> (hr)
1.00	2.61	0.83	1.24	5.32	10.0	28.7	8.17
5.00	13.05	4.00	6.20	26.60	50.0	143.3	40.85
228.20	752.20	189.40	357.37	1214.02	2282.0	6,537.9	1864.4
480.00	1252.8	398.4	595.2	2554.8	4800.0	13,752.0	3921.6
<b>979.19</b>	<b>2555.4</b>	<b>821.6</b>	<b>1214.0</b>	<b>5208.0</b>	<b>9791.90</b>	<b>28,053.8</b>	<b>8000.0</b>

*Table 6.3* summarised the results of *CDB* and *MultiVBD* columns in terms of amount of product in each cut, and total profit. For the *CBD* column three switching times  $t_1$ ,  $t_2$  and  $t_3$  were used for tasks 1, 2 and 3. From this table it can be noted that the *MultiVBD* column was found to be giving the same profit as in *CBD*. Therefore, appropriate comparison could not be made.

**Table 6.3:** Summary of the Results Using Profit Function.-1

Configuration	$D_1$	$R_1$	$D_2$	$t_1$	$B_f$	$t_2$	$C_{fc}$	$t_3$	$P$	$P$
	kmol	kmol	kmol	hr	kmol	hr	\$/hr	hr	\$/h	\$/yr
<i>CBD</i>	2.61	0.83	1.24	3.56	5.32	2.65	5.0	1.46	3.74	28,053.8
<i>MultiVBD</i>	2.61	0.83	1.24	7.67	5.32	-	5.0	-	3.74	28,053.8

Using the second profit function (Miladi and Mujtaba, 2004), the results in terms of optimum number of stages, vapour load, reflux ratio, cut time, annual capital cost, etc. are summarised in *Table 6.4*.

From *Table 6.4*, the total number of stages in *MultiVBD* column required is 40% more than that required for the conventional column *CBD*. However, the vapour load for the *MultiVBD* column is about 25% lower compared to *CBD* and the operating cost is 30% lower.

**Table 6.4:** Maximum Profit Using Profit Function -2

Configuration	$V$ Kmol	$Nt$	$OC_b$ \$/b	$ACC$ \$/yr	$P$ \$/b	$P$ \$/yr
<i>CBD</i>	3.0	10	0.55	35795	29.90	29270.8
<i>MultiVBD</i>	2.3	4, 6, 4	0.42	35111	30.72	30080.1
Reflux Ratio Profile for <i>CBD</i> :						
	Main-Cut 1 ( $D_1$ )		Off-Cut ( $R_1$ )		Main-Cut 2 ( $D_2$ )	
Reflux ratio	0.712	0.819	0.841	0.942	0.660	0.781
Switching Time (hr)	0.0-2.10	2.10-3.56	3.56-4.78	4.78-6.21	6.21-6.99	6.99-7.67

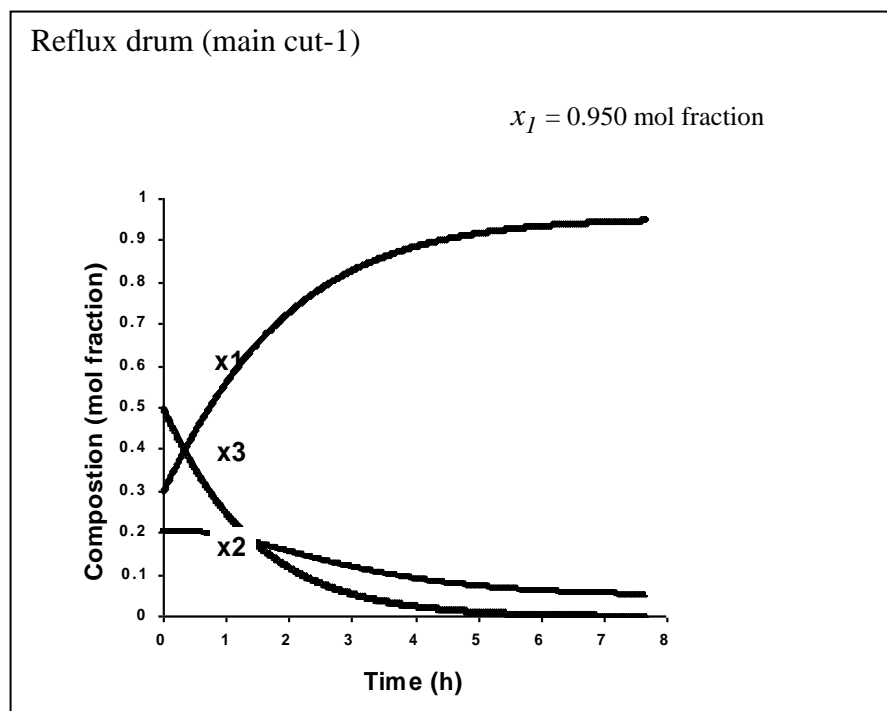
For conventional batch distillation column two time intervals were used for the reflux ratio ( $r$ ) in task 1 and task 3 and one time interval for the off-cut production. Three switching times are optimised for the whole multiperiod operation with the optimal reflux profiles in task 1 (main-cut 1) and in task 2 (off-cut 1) and in task 3 (main-cut 2) to ensure that the very high purities for requirements of component 1, 2 and off-cut 1.

The product demand and qualities (purities) of each main-cut and off-cut are achieved to meet on specifications.

Typical simulated composition profiles as a function of time are shown in *Figures 6.2 to 6.5.*, where  $x_1$  represent the first component in main cut-1,  $x_2$  represent the second component in main cut-1, and  $x_3$  represent the third component in main cut-1 and so on for the rest of products. As the end of batch time, compositions presented in *Table 6.5* will be achieved.

**Table 6.5:** Product Specifications of *MultiVBD* Column

Product Location	$x_1$	$x_2$	$x_3$
Main cut-1, (Reflux drum)	<b>0.950</b>	0.050	0.00
Off-cut-1, (Vessel-1)	<b>0.600</b>	0.400	0.00
Main cut-2, (Vessel-2)	0.027	<b>0.950</b>	0.023
Bottom Product, (Reboiler)	0.00	0.059	0.941



**Figure 6.2:** Composition of Main-Cut-1 of *MultiVBD* Column

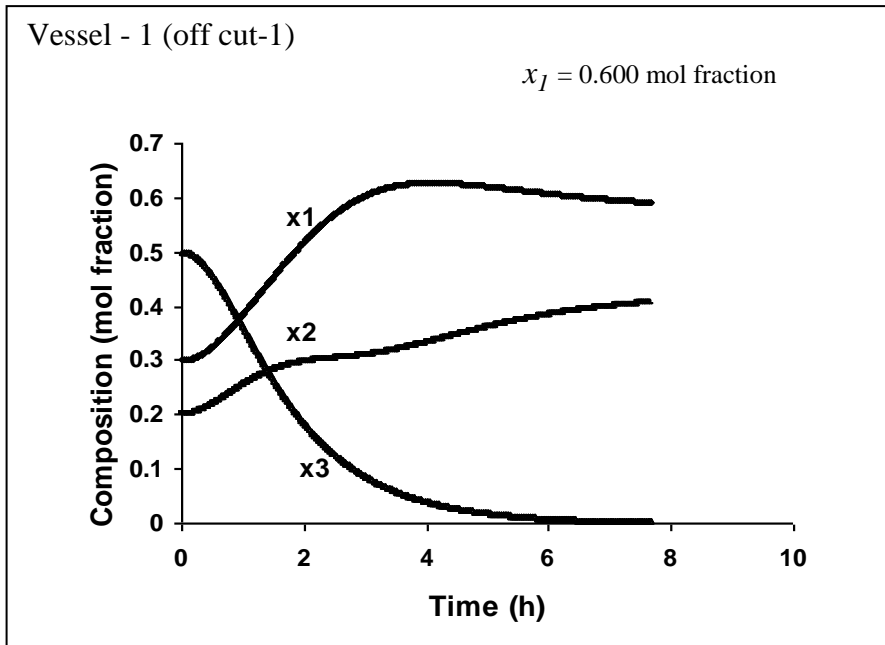


Figure 6.3: Composition of Off-Cut-1 of *MultiVBD* Column

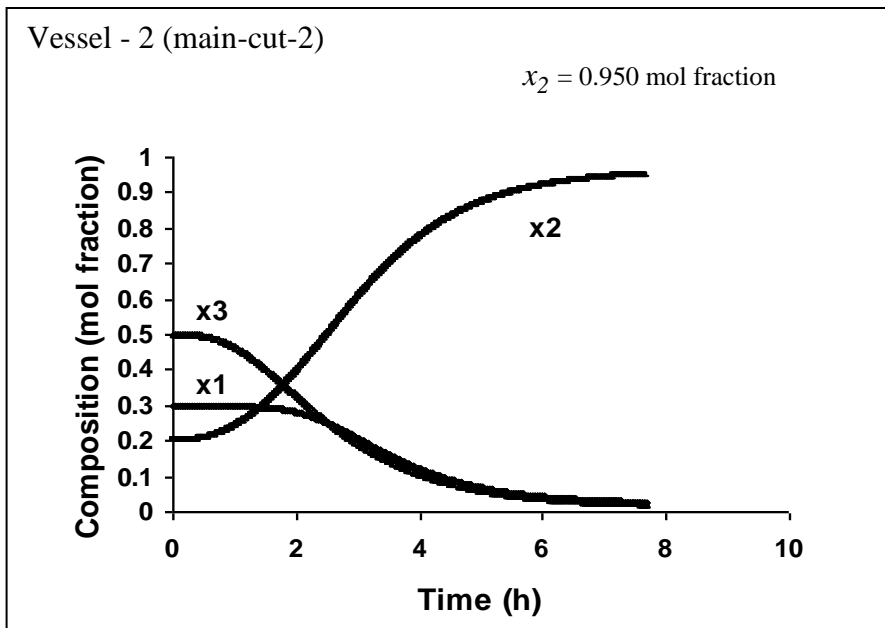
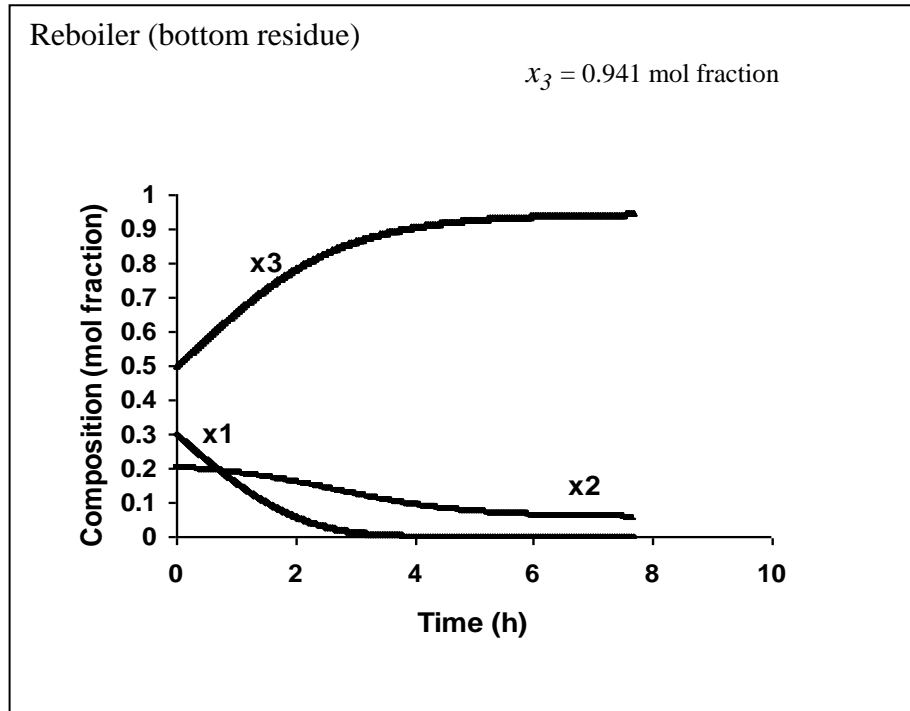


Figure 6.4: Composition of Main-Cut-2 of *MultiVBD* Column



**Figure 6.5:** Composition of Bottom Residue of *MultiVBD* Column

### 6.3 Conclusions

For the given separation task, the *MultiVBD* column was found to be more profitable than the *CBD* column for ternary separation. Also the operating cost (an indirect measure of the energy cost and environmental impact) for *MultiVBD* column was more than 30% lower compared to that by *CBD*.

Two different profit functions (profit \$/year) are used in this study to comparison. The first profit function (I) based on fixed operating cost (fixed design-5.0 \$/hr) in terms of number of plates and vapor flow rate and exclude set-up time and capital cost (*CC*). The *MultiVBD*

column was found to be giving the same net profit as in *CBD* column. Therefore, appropriate comparison could not be made.

The second profit function (II) based on the (variable design) in terms of number of plates and vapor flow rate, and operating cost and annualised capital cost. In this chapter the objective function was to maximise the profit per year. For the given separation task, the *MultiVBD* column was found to be more profitable than the *CBD* column. Also the operating cost (an indirect measure of the energy cost and environmental impact) for *MultiVBD* column was more than 30% lower compared to that by *CBD*. In all cases, product demand and quality are met on specifications.

# CHAPTER 7

## MULTICOMPONENT MULTIVESSEL BATCH DISTILLATION USING OTHER STNs

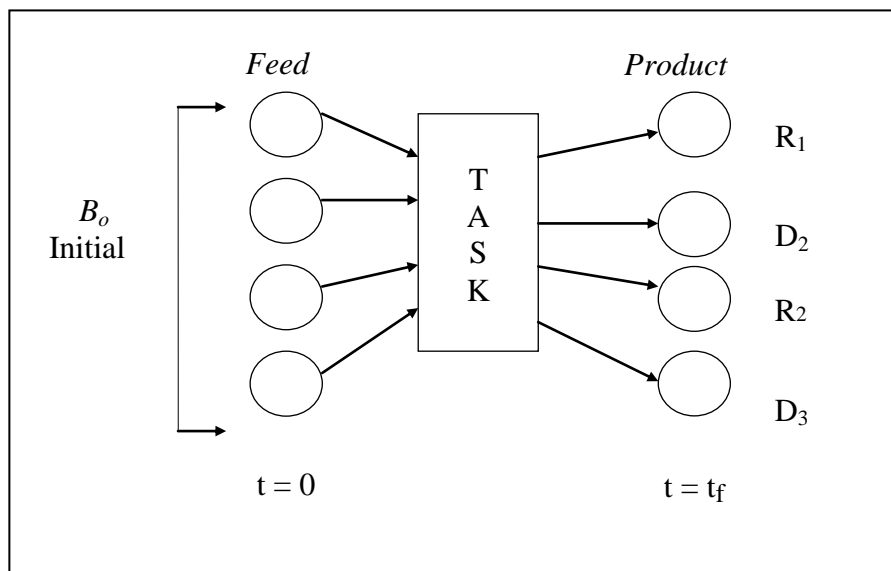
### 7.1 Introduction

Two State Tasks Networks (*STNs*) different to that presented in chapter 6 are considered in this chapter for ternary separation processes. The first State Task Network *STN-2* for *MultiVBD* is with each off-cut followed by a main-cut as shown in *Figure 7.1*, and the *STN-3* is with two main cuts and one off-cut in between as shown in *Figure 7.2*. *STN-2* is to achieve maximum overall profit with desired purities in terms of the key component mole fractions  $x^2_{D2}$  (for main-cut 1) and  $x^3_{D3}$  (for main-cut 2) with different composition of  $x^1_{R1}$  and the same recovery of component-1 in  $R_1$  (off-cut -1) in each case. In this specific operation the off cut-1 and off cut-2 ( $R_1$  and  $R_2$ ) are not desired products.

*STN-3* is to achieve maximum overall profit with desired purities in terms of the key components mole fractions  $x^1_{D1}$  for (main-cut 1) and  $x^3_{D2}$  for (main-cut 2) with different composition (product specifications) of  $x^1_{D1}$  and  $x^1_{R1}$  in each case study. In this specific operation the off cut-1 ( $R_1$ ) are not desired products.

## 7.2 Optimal Operation and Design with *STN-2*: (Case Study-1.1)

To process a ternary mixture with a known initial composition;  $x_{B_o}$ ,  $\langle 0.30, 0.20, 0.50 \rangle$ , the mixture is introduced into the *MultiVBD* column. The batch size is taken to be 10.0 kmol per batch, with specified purities in main cut-2 and main cut-3, in this specific operation the bottom residue product in vessel 4 ( $D_3$ ,  $x_{D_3}$ ) is a desired product. The *STN-2* in *Figure 7.1* is considered for the (ternary mixture with two off-cuts and two main-cuts).



**Figure 7.1:** *STN-2* with Each Off-Cut Followed by Main Cuts

Here, with consideration to the *STN-2* for ternary operations, the possible product profiles will be created with help of just the material balance calculations with the required product specifications and other given assumptions.

For *STN-2*, based on the material balance, the limits on the amount of products (that could be obtained from *STN-2*) will be calculated and presented, and the maximum profitable operation will be identified within these limits.

The objective function is to maximise the profit (per year), where:

$$\text{Profit (\$/y)} P = (C_1 D_1 + C_2 D_2 + C_3 R_1 - C_4 R_2 - C_5 B_0 - OC_b) \times N_B - ACC \quad (7.1)$$

where;  $C_1$ : Price of product  $D_1$  (kmol), and set to be  $C_1 = \$20.00$

$C_2$ : Price of product  $D_2$  (kmol), and set to be  $C_2 = \$20.00$

$C_3$ : Price of off-cut  $R_1$  (kmol), and set to be  $C_3 = \$0.0$

$C_4$ : Price of off-cut  $R_2$  (kmol), and set to be  $C_4 = \$0.0$

$C_5$ : Price of raw material (feed)  $B_0$  (kmol), and set to be  $C_5 = \$1.00$

Three different cases are considered based on fixing some of the variables such as recovery of (off cut-1) and varying some of the variables such as (off cut-1) compositions. It is assumed that the column operates for  $H = 8000$  hrs/yr with no idle time. The column configurations for optimisation studies are presented below;

Initial charge (*feed*), kmol  $B_0 = 10.0$

Feed composition,  $x_{B0} = \langle 0.30, 0.20, 0.50 \rangle$

Relative volatility,  $\alpha = \langle 8, 4, 1 \rangle$

Batch processing time, (hr)  $= 7.67$

Recovery of component-1 in (off-cut -1)  $= 97.5\%$ .

Product specifications, (*STN-2*)  $x_{D2}, x_{D3} = 0.95$  molefraction of component 2 & 3

The total numbers of the variable are:

- *Initials* (total initial charge;  $B_0$  kmol and compositions of each component at  $B_0; x^1_{B0}, x^2_{B0}, x^3_{B0}$ ).

- *Off-cut 1* (total amount of off-cut;  $R_1$  kmol and molefraction of each component at  $R_1; x^1_{R1}, x^2_{R1}, x^3_{R1}$ ).
- *Main-cut 1* (total amount of main-cut;  $D_2$  kmol and molefraction of each component at  $D_2; x^1_{D2}, x^2_{D2}, x^3_{D2}$ ).
- *Off-cut 2* (total amount of off-cut;  $R_2$  kmol and molefraction of each component at  $R_2; x^1_{R2}, x^2_{R2}, x^3_{R2}$ ).
- *Main-cut 2* or final bottom product (total amount of main-cut;  $D_3$  kmol and molefraction of each component at  $D_3; x^1_{D3}, x^2_{D3}, x^3_{D3}$ ).

The overall component mass balance:

$$\text{Component 1: } B_0 x^1_{B0} = R_1 x^1_{R1} + D_2 x^1_{D2} + R_2 x^1_{R2} + D_3 x^1_{D3} \quad (7.2)$$

$$\text{Component 2: } B_0 x^2_{B0} = R_1 x^2_{R1} + D_2 x^2_{D2} + R_2 x^2_{R2} + D_3 x^2_{D3} \quad (7.3)$$

The overall total mass balance:

$$B_0 = R_1 + D_2 + R_2 + D_3 \quad (7.4)$$

$$\text{Constraint } \sum x_{R1} = 1 \quad (7.5)$$

$$\sum x_{D2} = 1 \quad (7.6)$$

$$\sum x_{R2} = 1 \quad (7.7)$$

$$\sum x_{D3} = 1 \quad (7.8)$$

- Given: Initials:  $B_0, x^1_{B0}, x^2_{B0}, x^3_{B0} \longrightarrow 4$  specifications
- Product purity:  $x^2_{D2}, x^3_{D3} \longrightarrow 2$  desired specifications

### 7.2.1 Sample Calculations

With consideration to the *STNs* for ternary batch distillation operations, the possible product profiles will be created with the help of just the material balance calculations with the required product specifications and other given assumptions. For *STN*, based on the material balance, the limits on the amount of products (that could be obtained from *STN*) will be calculated and presented, and the maximum profitable operation (per batch) will be determined within these limits. The maximum profit per batch will then be used to calculate the total profit.

Given  $B_0$  (feed) = 10 kmol,  $x^1_{B0} = 0.30$ ,  $x^2_{B0} = 0.20$ ,  $x^3_{B0} = 0.50$

Specified product purities are;

$$x^2_{D2} = 0.95, x^3_{D3} = 0.95$$

Assumptions:  $x^3_{R1} = 0.0$ ,  $x^3_{D2} = 0.0$ ,  $x^1_{R2} = 0.0$ ,  $x^1_{D3} = 0.0$ , and

$R_2$  is assumed to be vary in each case study.

Note: although,  $x^3_{R1} = 0.0$ ,  $x^1_{D3} = 0.0$  and  $x^1_{R2}$  may be achieved with appropriate  $N$  and  $V$ , but  $D_2$  can affect the overall profitability equation (7.1). Here the sensitivity of the choice of  $D_2$  on the operation and profitability will be assumed.

Solution of equations (7.2) - (7.8) with the above specifications and with random values of  $D_2$  and assumptions are summarized in *Table 7.1*. For each value of  $D_2$ , the limits on the amount of products (i.e.  $D_2$  and  $D_3$ ) for this *STN* are shown in *Table 7.1*.

From *Table 7.1*, six different cases with different amount of products are assumed based on material balance and appropriate  $N$  and  $V$  to achieve the overall profitability. The following conclusions are drawn:

1. The maximum possible value of  $D_2$  is shown 1.48 kmol, which is calculated based on the assumption of  $R_2$ .
2. The limits on the amount of products of this *STN* (*Figure 7.1*) could be summarised as follows:

$$(R_{1, \min} = R_{1, \max}) = (3.25, 3.25), R_1 \text{ is off-cut-1 (kmol/batch).}$$

$$(D_{2, \min}, D_{2, \max}) = (0.90, 1.48), D_2 \text{ is main-cut-1 (kmol/batch).}$$

$$(R_{2, \min}, R_{2, \max}) = (0.01, 1.00), R_2 \text{ is off-cut-2 (kmol/batch).}$$

$$(D_{3, \min}, D_{3, \max}) = (4.85, 5.26), D_3 \text{ is main-cut-2 (kmol/batch).}$$

3. Off-cut 2 ( $R_2$ ) increases as both  $D_2$ ,  $D_3$  decrease.

**Table 7.1:** Possible Product Profiles for *STN-2 (Case-1.1)* Based on Mass Balance Only

Case	Off-Cut-1			Main-Cut-1			Off-Cut -2			Main-Cut-2		
	$R_1$	$x^1_{R1}$	$x^2_{R1}$	$D_2$	$x^1_{D2}$	$x^2_{D2}$	$R_2$	$x^2_{R2}$	$x^3_{R2}$	$D_3$	$x^2_{D3}$	$x^3_{D3}$
A	3.25	<b>0.900</b>	0.100	1.48	<b>0.050</b>	0.950	<b>0.01</b>	0.600	0.400	5.26	<b>0.050</b>	0.950
B	3.25	<b>0.900</b>	0.100	1.42	<b>0.050</b>	0.950	<b>0.10</b>	0.600	0.400	5.23	<b>0.050</b>	0.950
C	3.25	<b>0.900</b>	0.100	1.39	<b>0.050</b>	0.950	<b>0.15</b>	0.600	0.400	5.21	<b>0.050</b>	0.950
D	3.25	<b>0.900</b>	0.100	1.36	<b>0.050</b>	0.950	<b>0.20</b>	0.600	0.400	5.19	<b>0.050</b>	0.950
E	3.25	<b>0.900</b>	0.100	1.19	<b>0.050</b>	0.950	<b>0.50</b>	0.600	0.400	5.06	<b>0.050</b>	0.950
F	3.25	<b>0.900</b>	0.100	0.90	<b>0.050</b>	0.950	<b>1.00</b>	0.600	0.400	4.85	<b>0.050</b>	0.950

## 7.2.2 Profit Calculations

The calculation procedure is described earlier. Using the product profiles of *Table 7.1* it was found that *Case-A* gives the maximum profit per year. The results with cases *B*, *C* and *D* are presented in (*Table 7.2*). Note, product specifications in (*Table 7.1*) will dictate product profile per batch and will dictate the total amount of product that can be produced over a year. Also note, changing one of the product demands will change the amount of production of other product and may lead to over or underproduction of that product.

*Table 7.2* summarise the results as follows:

- Total number of batches per year  $N_B = 979.19$  in terms of fixed time = 7.67hr.
- $(CD_2, CD_3, CB_0)$  are the prices of main cuts and cost of feed (material-\$).
- All the product quality is met on specifications
- Off-cut 2 ( $R_2$ ) increases as both  $D_2, D_3$  decrease.
- The product of  $R_1$  and  $R_2$  are not desired products
- The net profit increases with increase the amount of  $D_2, D_3$ .

The number of plates for each column section was optimised (equation 4.6 in chapter-4) together with vapour load to achieve the required specifications in each case. For each case, the results giving the maximum profit are shown in italic. For example for Case A ( $D_2 = 1.48\text{kmol}$ ),  $N = 13$  with  $V = 2.82 \text{ kmol/hr}$  give the maximum profit of 83453.0 \$/yr compared to the profits obtained in Cases *B*, *C* and *D*. The main cut products  $D_2, D_3$  can affect the overall profitability (equation 7.1)

**Table 7.2:** Optimal Operation and Design for *STN-2 (Case-1.1)*

CASE	OFF-CUT-1				MAIN-CUT-1				OFF-CUT-2				MAIN-CUT-2				
	$R_1$	$X^1_{R1}$	$X^2_{R1}$	$X^3_{R1}$	$D_2$	$X^1_{D2}$	$X^2_{D2}$	$X^3_{D2}$	$R_2$	$X^1_{R2}$	$X^2_{R2}$	$X^3_{R2}$	$D_3$	$X^1_{D3}$	$X^2_{D3}$	$X^3_{D3}$	
A	3.25	0.905	0.093	0.002	1.48	0.041	<b>0.950</b>	0.009	0.01	0.004	0.754	0.241	5.26	0.0	0.050	<b>0.950</b>	
B	3.25	0.913	0.084	0.002	1.42	0.025	<b>0.950</b>	0.024	0.10	0.005	0.761	0.234	5.23	0.0	0.050	<b>0.950</b>	
C	3.25	0.913	0.084	0.002	1.39	0.025	<b>0.950</b>	0.024	0.15	0.005	0.756	0.243	5.21	0.0	0.050	<b>0.950</b>	
D	3.25	0.913	0.079	0.007	1.36	0.028	<b>0.950</b>	0.021	0.20	0.005	0.752	0.242	5.19	0.0	0.050	<b>0.950</b>	
<i>PROFIT SUMMARY</i>																	
CASE	$CD_2$	$CD_3$	$C_{B0}$	$R_1$	$D_2$	$R_2$	$D_3$	$V$	$N$	$T,$	$NB$	$OC$	$CC$	$ACC$	$P$	$P$	$P$
	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	kmol/hr		hr	yr	\$/b	\$/b	\$/yr	\$/hr	\$/b	\$/yr
A	20.0	20.0	1.0	3.25	<b>1.48</b>	0.01	<b>5.26</b>	<b>2.82</b>	<b>8, 3, 2</b>	7.67	979.1	0.52	39.06	38242.6	10.43	85.23	<b>83453.0</b>
B	20.0	20.0	1.0	3.25	1.42	0.10	5.23	2.68	<b>9, 2, 2</b>	7.67	979.1	0.49	37.93	37142.9	10.35	84.58	82815.3
C	20.0	20.0	1.0	3.25	1.39	0.15	5.21	2.68	<b>9, 2, 2</b>	7.67	979.1	0.48	37.93	37142.9	10.23	83.58	81836.1
D	20.0	20.0	1.0	3.25	1.36	0.20	5.19	2.65	<b>10, 2, 2</b>	7.67	979.1	0.43	37.69	36904.2	10.14	82.82	81101.0

### 7.3 Optimal Operation and Design with *STN-2*: (*Case Study-1.2*)

Referring to *STN-2* in *Figure 7.1* (ternary mixture with two off-cuts and two main-cuts), and following with the same procedure of that calculations of (*Case study-1.1*) using the recovery of component-1 in (off-cut -1) is 97.5% with composition of  $x^1_{R1} = 0.950$  mole fraction to achieve maximum profit. For this *STN*, the optimum product profiles and maximum profit achieved are presented in *Table 7.3*, and *Table 7.4*.

Note: although,  $x^3_{R1} = 0.0$ ,  $x^1_{D3} = 0.0$  and  $x^1_{R2}$  may be achieved with appropriate  $N$  and  $V$ , but  $D_2$  can affect the overall profitability equation (7.1). Here the sensitivity of the choice of  $D_2$  on the operation and profitability will be assumed.

Solution of equations (7.2) - (7.8) with the above specifications and with random values of  $D_2$  and assumptions are summarized in *Table 7.3*.

For each value of  $D_2$ , the limits on the amount of products (i.e.  $D_2$  and  $D_3$ ) for this *STN* are shown in *Table 7.3*.

From *Table 7.3*, six different cases with different amount of products are assumed based on material balance and appropriate  $N$  and  $V$  to achieve the overall profitability.

The following conclusions are drawn:

- 1 The maximum possible value of  $D_2$  is shown 1.65 kmol, which is calculated based on the assumption of  $R_2$ .
- 2 The limits on the amount of products of *STN* (*Figure 6.1*) could be summarised as follows:

$$(R_{1, \min} = R_{1, \max}) = (3.08, 3.08), R_1 \text{ is off-cut-1 (kmol/batch).}$$

$$(D_{2, \min}, D_{2, \max}) = (1.07, 1.65), D_2 \text{ is main-cut-1 (kmol/batch).}$$

$(R_{2, \min}, R_{2, \max}) = (0.01, 1.00)$ ,  $R_2$  is off-cut-2 (kmol/batch).

$(D_{3, \min}, D_{3, \max}) = (4.85, 5.26)$ ,  $D_3$  is main-cut-2 (kmol/batch).

- 3 Off-cut 2 ( $R_2$ ) increases as both  $D_2, D_3$  decrease.

**Table 7.3:** Possible Product Profiles for *STN-2 (Case-1.2)* Based on Mass Balance Only

Case	Off-Cut-1			Main-Cut-1			Off-Cut -2			Main-C u t-2		
	$R_1$	$X^1_{R1}$	$X^2_{R1}$	$D_2$	$X^1_{D2}$	$X^2_{D2}$	$R_2$	$X^2_{R2}$	$X^3_{R2}$	$D_3$	$X^2_{D3}$	$X^3_{D3}$
A	3.08	<b>0.950</b>	0.050	1.65	<b>0.050</b>	0.950	<b>0.01</b>	0.600	0.400	5.26	<b>0.050</b>	0.950
B	3.08	<b>0.950</b>	0.050	1.59	<b>0.050</b>	0.950	<b>0.10</b>	0.600	0.400	5.23	<b>0.050</b>	0.950
C	3.08	<b>0.950</b>	0.050	1.56	<b>0.050</b>	0.950	<b>0.15</b>	0.600	0.400	5.21	<b>0.050</b>	0.950
D	3.08	<b>0.950</b>	0.050	1.53	<b>0.050</b>	0.950	<b>0.20</b>	0.600	0.400	5.19	<b>0.050</b>	0.950
E	3.08	<b>0.950</b>	0.050	1.36	<b>0.050</b>	0.950	<b>0.50</b>	0.600	0.400	5.06	<b>0.050</b>	0.950
F	3.08	<b>0.950</b>	0.050	1.07	<b>0.050</b>	0.950	<b>1.00</b>	0.600	0.400	4.85	<b>0.050</b>	0.950

### 7.3.1 Profit Calculations

The calculation procedure is described earlier as the same as in (*Case study -1.1*). Using the product profiles of *Table 7.3* it was found that *Case-A* gives the maximum profit per year. The results with cases *B*, *C*, and *D* are presented in *Table 7.4*. Note, product specifications in (*Table 7.3*) will dictate product profile per batch and will dictate the total amount of product that can be produced over a year. Also note, changing one of the product demands will change the amount of production of other product and may lead to over or underproduction of that product.

*Table 7.4* summarise the results as follows:

- Total number of batches per year  $NB = 979.19$  in terms of fixed time =7.67hr.
- $(CD_2, CD_3, CB_0)$  are the prices of main cuts and cost of feed (material-\$).
- All the product quality is met on specifications
- The product of  $R_1$  and  $R_2$  are not desired products.
- Off-cut 2 ( $R_2$ ) increases as both  $D_2, D_3$  decrease.
- The net profit increases with increase the amount of  $D_2, D_3$ .

The number of plates for each column section was optimised together with vapour load to achieve the required specifications in each case.

For each case, the results giving the maximum profit are shown in italic. For example for Case A ( *$D_2 = 1.65\text{kmol}$* ),  *$N = 15$*  with  *$V = 2.38 \text{ kmol/hr}$*  give the maximum profit of 88217.0 \$/yr compared to the profits obtained in Cases *B*, *C* and *D*.

The main cut products  $D_2, D_3$  can affect the overall profitability (equation 7.1)

**Table 7.4:** Optimal Operation and Design for *STN-2* (Case-1.2)

CASE	OFF-CUT-1				MAIN-CUT-1				OFF-CUT-2				MAIN-CUT-2			
	$R_1$	$X^1_{R1}$	$X^2_{R1}$	$X^3_{R1}$	$D_2$	$X^1_{D2}$	$X^2_{D2}$	$X^3_{D2}$	$R_2$	$X^1_{R2}$	$X^2_{R2}$	$X^3_{R2}$	$D_3$	$X^1_{D3}$	$X^2_{D3}$	$X^3_{D3}$
A	3.08	0.963	0.034	0.002	1.65	0.024	<b>0.950</b>	0.025	0.01	0.005	0.755	0.239	5.26	0.00	0.050	<b>0.950</b>
B	3.08	0.956	0.041	0.003	1.59	0.035	<b>0.950</b>	0.014	0.10	0.003	0.744	0.252	5.23	0.0	0.050	<b>0.950</b>
C	3.08	0.961	0.035	0.003	1.56	0.023	<b>0.950</b>	0.026	0.15	0.005	0.753	0.242	5.21	0.0	0.050	<b>0.950</b>
D	3.08	0.961	0.035	0.003	1.53	0.023	<b>0.950</b>	0.027	0.20	0.005	0.749	0.246	5.19	0.0	0.050	<b>0.950</b>

<i>PROFIT SUMMARY</i>																	
CASE	$CD_2$	$CD_3$	$CB_O$	$R_1$	$D_2$	$R_2$	$D_3$	$V$	$N$	$T$	$N_B$	$OC$	$CC$	$ACC$	$P$	$P$	$P$
	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	kmol/hr		hr	yr	\$/b	\$/b	\$/yr	\$/hr	\$/b	\$/yr
A	20.0	20.0	1.0	3.08	<b>1.65</b>	0.01	<b>5.26</b>	<b>2.38</b>	<b>11, 2, 2</b>	7.67	979.1	0.43	37.67	36887.0	11.03	90.1	<b>88217.0</b>
B	20.0	20.0	1.0	3.08	1.59	0.10	5.23	2.37	11, 2, 2	7.67	979.1	0.43	37.58	36798.9	10.82	88.38	86544.3
C	20.0	20.0	1.0	3.08	1.56	0.15	5.21	2.46	12, 2, 2	7.67	979.1	0.45	39.50	38674.2	10.46	85.45	83673.7
D	20.0	20.0	1.0	3.08	1.53	0.20	5.19	2.45	12, 2, 2	7.67	979.1	0.45	39.41	38585.1	10.35	84.54	82785.4

## 7.4 Optimal Operation and Design with *STN-2*: (Case Study-1.3)

Referring to *SNT-2* in *Figure 7.1* (ternary mixture with two off-cuts and two main-cuts), and following with the same procedure of that calculations (*Case study-1.1*) using of the recovery of component-1 in (off-cut -1) is 97.5% and with composition of  $x^1_{R1} = 0.970$  mole fraction to achieve maximum profit. For this *STN*, the optimum product profiles and maximum profit achieved are presented in *Table 7.5*, and *Table 7, 6*.

Note: although,  $x^3_{R1} = 0.0$ ,  $x^1_{D3} = 0.0$  and  $x^1_{R2}$  may be achieved with appropriate  $N$  and  $V$ , but  $D_2$  can affect the overall profitability equation (7.1). Here the sensitivity of the choice of  $D_2$  on the operation and profitability will be assumed.

Solution of equations (7.2) - (7.8) with the above specifications and with random values of  $D_2$  and assumptions are summarized in *Table 7.5*. For each value of  $D_2$ , the limits on the amount of products (i.e.  $D_2$  and  $D_3$ ) for this *STN* are shown in *Table 7.5*.

From *Table 7.5*, six different cases with different amount of products are assumed based on material balance and appropriate  $N$  and  $V$  to achieve the overall profitability. The following

From *Table 6.5*, the following conclusions can be drawn:

- 1 The maximum possible value of  $D_2$  is shown 1.72 kmol, which is calculated based on the assumption  $R_2$ .
- 2 The limits on the amount of products of this *STN* (*Figure 7.1*) could be summarised as follows:

$$(R_{1, \min} = R_{1, \max}) = (3.01, 3.01), R_1 \text{ is off-cut-1 (kmol/batch).}$$

$$(D_{2, \min}, D_{2, \max}) = (1.15, 1.72), D_2 \text{ is main-cut-1 (kmol/batch).}$$

$(R_{2, \min}, R_{2, \max}) = (0.01, 1.00)$ ,  $R_2$  is off-cut-2 (kmol/batch).

$(D_{3, \min}, D_{3, \max}) = (4.85, 5.26)$ ,  $D_3$  is main-cut-2 (kmol/batch).

- 3 Off-cut 2 ( $R_2$ ) increases as both  $D_2, D_3$  decrease.

**Table 7.5:** Possible Product Profiles for *STN-2 (Case-1.3)* Based on Mass Balance Only

Case	Off-Cut-1			Main-Cut-1			Off-Cut-2			Main-Cu t-2		
	$R_1$	$X^1_{R1}$	$X^2_{R1}$	$D_2$	$X^1_{D2}$	$X^2_{D2}$	$R_2$	$X^2_{R2}$	$X^3_{R2}$	$D_3$	$X^2_{D3}$	$X^3_{D3}$
A	3.01	<b>0.970</b>	0.030	1.72	<b>0.050</b>	0.950	<b>0.01</b>	0.600	0.400	5.26	<b>0.050</b>	0.950
B	3.01	<b>0.970</b>	0.030	1.66	<b>0.050</b>	0.950	<b>0.10</b>	0.600	0.400	5.23	<b>0.050</b>	0.950
C	3.01	<b>0.970</b>	0.030	1.63	<b>0.050</b>	0.950	<b>0.15</b>	0.600	0.400	5.21	<b>0.050</b>	0.950
D	3.01	<b>0.970</b>	0.030	1.60	<b>0.050</b>	0.950	<b>0.20</b>	0.600	0.400	5.19	<b>0.050</b>	0.950
E	3.01	<b>0.970</b>	0.030	1.43	<b>0.050</b>	0.950	<b>0.50</b>	0.600	0.400	5.06	<b>0.050</b>	0.950
F	3.01	<b>0.970</b>	0.030	1.14	<b>0.050</b>	0.950	<b>1.00</b>	0.600	0.400	4.85	<b>0.050</b>	0.950

### 7.4.1 Profit Calculations

The calculation procedure is described earlier as the same as in (*Case study-1.1*). Using the product profiles of *Table 7.5* it was found that *Case-A* gives the maximum profit per year. The results with cases *A*, *B*, *C* and *D* are presented in (*Table 7.6*). Note, product specifications in (*Table 7.5*) will dictate product profile per batch and will dictate the total amount of product that can be produced over a year. Also note, changing one of the product demands will change the amount of production of other product and may lead to over or underproduction of that product.

*Table 7.6* summarise the results as follows:

- Total number of batches per year  $NB = 979.19$  in terms of fixed time =7.67hr.
- $(CD_2, CD_3, CB_0)$  are the prices of main cuts and cost of feed (material-\$).
- All the product quality is met on specifications
- The product of  $R_1$  and  $R_2$  are not desired products.
- Off-cut 2 ( $R_2$ ) increases as both  $D_2, D_3$  decrease.
- The net profit increases with increase the amount of  $D_2, D_3$ .

The number of plates for each column section was optimised together with vapour load to achieve the required specifications in each case.

For each case, the results giving the maximum profit are shown in italic. For example for Case *A* ( $D_2 = 1.72$  kmol),  $N = 18$  with  $V = 2.42$  kmol/hr give the maximum profit of 86032.0 \$/yr compared to the profits obtained in Cases *B*, *C* and *D* due to low vapour load.

The main cut products  $D_2, D_3$  can affect the overall profitability (equation 7.1)

**Table 7.6:** Optimal Operation and Design for *STN-2* (*Case-1.3*)

CASE	OFF-CUT-1				MAIN-CUT-1				OFF-CUT-2				MAIN-CUT-2			
	$R_1$	$X^1_{R1}$	$X^2_{R1}$	$X^3_{R1}$	$D_2$	$X^1_{D2}$	$X^2_{D2}$	$X^3_{D2}$	$R_2$	$X^1_{R2}$	$X^2_{R2}$	$X^3_{R2}$	$D_3$	$X^1_{D3}$	$X^2_{D3}$	$X^3_{D3}$
A	3.01	0.973	0.024	0.003	1.72	0.037	<b>0.950</b>	0.013	0.01	0.003	0.745	0.251	5.26	0.0	0.050	<b>0.950</b>
B	3.01	0.979	0.019	0.001	1.66	0.025	<b>0.950</b>	0.024	0.10	0.005	0.755	0.234	5.23	0.0	0.050	<b>0.950</b>
C	3.01	0.980	0.018	0.001	1.63	0.026	<b>0.950</b>	0.024	0.15	0.005	0.751	0.243	5.21	0.0	0.050	<b>0.950</b>
D	3.01	0.980	0.017	0.002	1.60	0.025	<b>0.950</b>	0.024	0.20	0.005	0.744	0.251	5.19	0.0	0.046	<b>0.953</b>

*PROFIT SUMMARY*

CASE	$CD_2$	$CD_3$	$CB_0$	$R_1$	$D_2$	$R_2$	$D_3$	$V$	$N$	$T$	$NB$	$OC$	$CC$	$ACC$	$P$	$P$	$P$
	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	kmol/hr		hr	yr	\$/b	\$/b	\$/yr	\$/hr	\$/b	\$/yr
A	20.0	20.0	1.0	3.01	<b>1.72</b>	0.01	<b>5.26</b>	<b>2.42</b>	<b>13,3,2</b>	7.67	979.1	0.44	41.29	40435.7	10.75	87.86	<b>86032.0</b>
B	20.0	20.0	1.0	3.01	1.66	0.10	5.23	2.59	14,2,2	7.67	979.1	0.48	42.90	42010.5	10.30	84.02	82272.4
C	20.0	20.0	1.0	3.01	1.63	0.15	5.21	2.60	14,2,2	7.67	979.1	0.48	42.90	42101.8	10.20	83.40	81591.8
D	20.0	20.0	1.0	3.01	1.60	0.20	5.19	2.61	14,2,2	7.67	979.1	0.49	43.37	42192.9	10.06	82.23	80519.7

## 7.5 Conclusions

The State Task Network defined as *STN* in terms of option and number of cuts is considered for ternary distillation. Overall product demands, product quality and feed specifications allow calculation of product profiles (amount of each product) of each batch a priori using steady state mass balance calculations. Product profiles were generated based on fixing some of the variables such as amount of off cuts  $R$  and composition of off cuts  $x_R$

The recovery of component 1 in the off cut  $R_1$  is fixed at 97.5%, while the composition of off cut -1 ( $x^1_{R1}$ ) is left as a decision variable. The effect of off cut compositions on the design and operation is carried out as shown in (*Tables- 7.2, 7.4, 7.6*)

The objective was to improve overall profit (\$/yr) with desired purities in terms of the key component mole fractions  $x^2_{D2}$  (for main-cut 1) and  $x^3_{D2}$  (for main-cut 2) in each case. In this specific operation the off cut-1 and off cut-2 ( $R_1$  and  $R_2$ ) are not desired products. In this *STN-2*, the optimal profit is achieved in (*case 1.2 A*) 87146.9 \$/yr with optimum  $N = 15$  stages and  $V = 2.38$  kmol/hr.

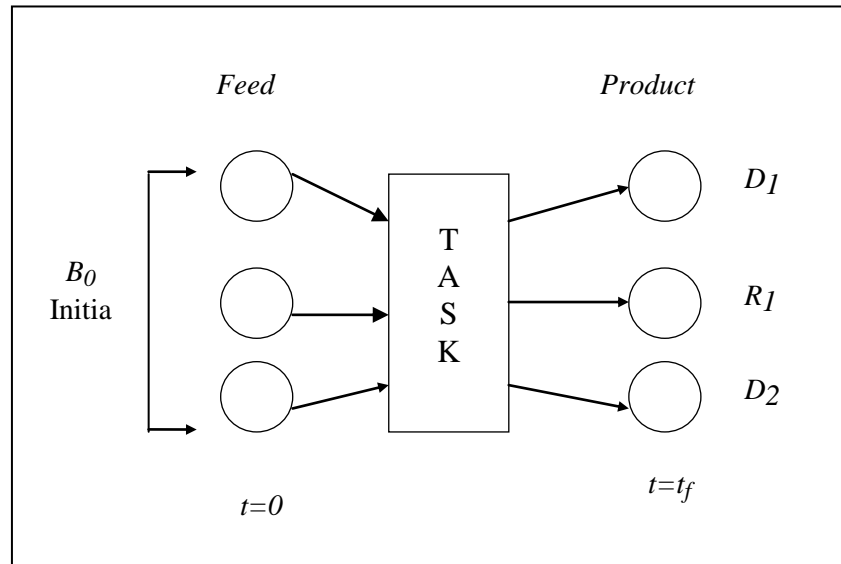
The results also show the operating cost per batch, annualised capital cost, profit per batch and per year, where the *OC*, *ACC*, and *CC* for this case (*1.2 A*) is lower compared to the other cases (*1.1 A*, and *1.3 A*) by 17.3 % and 2.3% respectively, also the profit is improved with off cut composition  $x^1_{R1}$  at 95%

Note, from the results that the column to have high vapour loading and high number of trays would expense of capital cost and utility cost and leading to lower profit.

## 7.6 Optimal Operation and Design with *STN-3*: (Case Study-2.1)

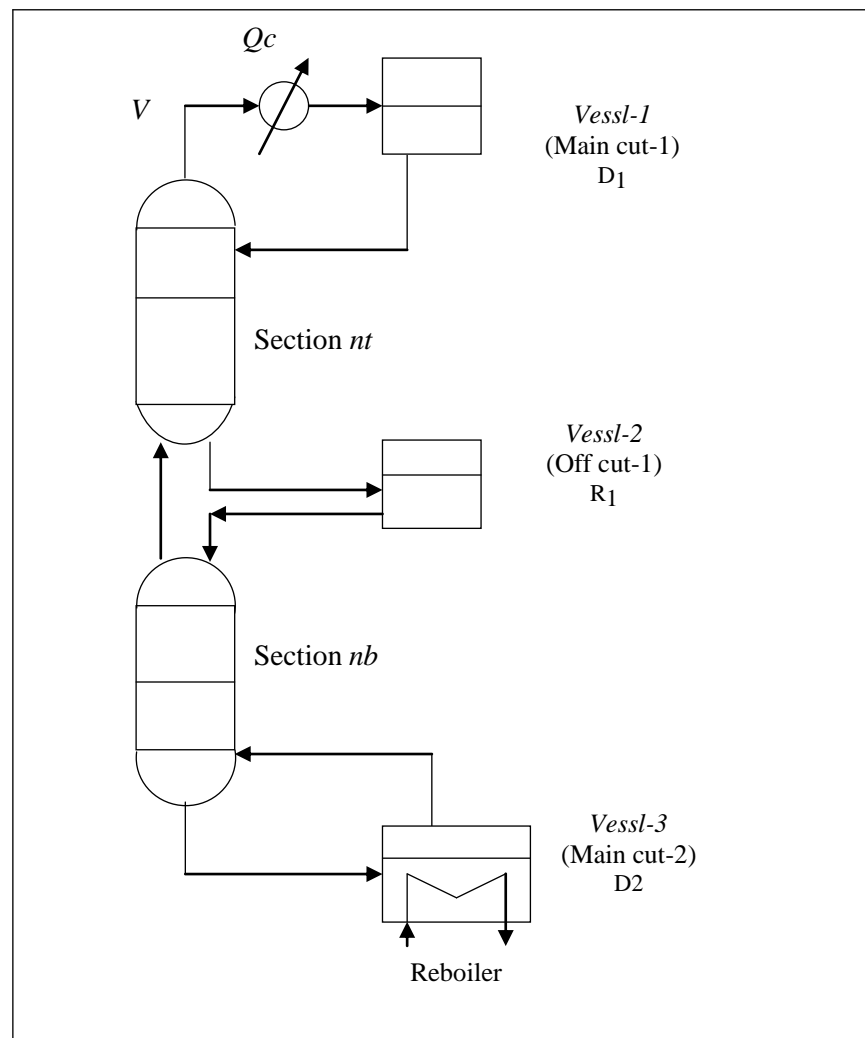
The second State Tasks Network defined as *STN-3* (Figure 7.2) with two main-cuts and one off-cut in between. The *MultiVBD* column with two column sections for ternary mixture (Figure 7.3) is considered to produce 3 products (two main-cuts and one off-cut in each case).

The *STN-3* is to achieve maximum overall profit with desired purities in terms of the key component mole fractions  $x^1_{D1}$  (for main-cut 1) and  $x^3_{D2}$  (for main-cut 2) with different composition of  $x^1_{R1}$  in each case study. In this specific operation the off cut-1 ( $R_1$ ) is not desired product. The material balance for *STN-3* is same as in previous cases *STN-2* but with only 3 products.



**Figure 7.1:** *STN-3* with Two Main Cuts and One Off-Cut in Between

To process a ternary mixture with a known initial composition;  $x_{B0}$ ,  $\langle 0.30, 0.20, 0.50 \rangle$ , the mixture is introduced into the *MultiVBD* column and distributed among the vessels. The batch size is taken to be 10.0 kmol per batch, with specified purities in main cut-1 and 2. The batch processing time is 7.67hr with total number of batches per year is 979.19.



**Figure 7.3:** Multivessel Batch Distillation with Two Column Sections

Here, with consideration to the *STN-3* for ternary batch distillation operations, the possible product profiles will be created with help of just the material balance calculations with the required product specifications and other given assumptions.

For *STN*, based on the material balance, the limits on the amount of products (that could be obtained from *STN*) will be calculated and presented, and the maximum profitable operation will be identified within these limits.

The objective function is to maximise the profit (per year) and used the same profit function in previous of *STN-2*. It is assumed that the column operates for  $H = 8000$  hrs/yr with no idle time

The column configurations for optimisation studies are presented below;

Initial charge (*feed*), kmol  $B_0 = 10.0$

Feed composition,  $x_{B0} = \langle 0.30, 0.20, 0.50 \rangle$

Relative volatility,  $(\alpha) = \langle 8, 4, 1 \rangle$

Batch processing time, (hr)  $= 7.67$

Product specifications, (*STN-3*)  $x_{D1}, x_{D2} = 0.95$  molefraction of component 1 & 2

The total numbers of the variables are:

- *Initials* (total initial charge;  $B_0$  kmol and compositions of each component at  $B_0$ ;  $x^1_{B0}, x^2_{B0}, x^3_{B0}$ )
- *Main-cut 1* (total amount of main-cut;  $D_1$  kmol and molefraction of each component at  $D_1$ ;  $x^1_{D1}, x^2_{D1}, x^3_{D1}$ ).

- *Off-cut 1* (total amount of off-cut;  $R_1$  kmol and molefraction of each component at  $R_1$ ;  $x^1_{R1}, x^2_{R1}, x^3_{R1}$ ).
- *Main-cut 2* or final bottom product (total amount of main-cut;  $D_2$  kmol and molefraction of each component at  $D_2$ ;  $x^1_{D2}, x^2_{D2}, x^3_{D2}$ ).

The overall component mass balance:

$$\text{Component 1: } B_0 x^1_{B0} = D_1 x^1_{D1} + R_1 x^1_{R1} + D_2 x^1_{D2} \quad (7.9)$$

$$\text{Component 2: } B_0 x^2_{B0} = D_1 x^2_{D1} + R_1 x^2_{R1} + D_2 x^2_{D2} \quad (7.10)$$

The overall total mass balance:

$$B_0 = D_1 + R_1 + D_2 \quad (7.11)$$

$$\text{Constraint: } \sum x_{D1} = 1 \quad (7.12)$$

$$\sum x_{R1} = 1 \quad (7.13)$$

$$\sum x_{D2} = 1 \quad (7.14)$$

Given:      Initials:       $B_0 x^1_{B0}, x^2_{B0}, x^3_{B0}$        $\longrightarrow$       4 specifications

                 Product purity:       $x^1_{D1}, x^2_{D2}$        $\longrightarrow$       2 desired specifications

### 7.6.1 Sample Calculations

Given  $B_0 = 10 \text{ kmol}$ ,  $x^1_{B0} = 0.30$ ,  $x^2_{B0} = 0.20$ ,  $x^3_{B0} = 0.50$

Specified product purities are;

$$x^1_{D1} = 0.95, x^3_{D2} = 0.95$$

Assumptions  $x^3_{D1} = 0.0$ ,  $x^3_{R1} = 0.0$ ,  $x^1_{D2} = 0.0$ ,

Let;  $x^1_{R1} = 0.40, 0.10$ , and  $0.05$ , respectively on each case study.

For the given specifications and assumptions, the solutions of equations (7.9 - 7.14) are summarised in *Table 7.7*, and the limits on the amount of products of this *STN* are presented.

From *Table 7.7*, the following conclusions can be drawn:

1. The maximum possible value of  $D_2$  is shown 5.26 kmol, which is calculated based on the assumption that all of component 3 will be removed in main-cut 2.
2. The limits on the amount of products of this *STN* (*Figure 7.2*) could be summarised as follows:

$$(D_{1, \min}, D_{1, \max}) = (1.58, 2.01)$$

$$(R_{1, \min}, R_{1, \max}) = (2.73, 3.75)$$

$$(D_{2, \min}, D_{2, \max}) = (4.67, 5.26)$$

3. Off-cut 1 ( $R_1$ ) increases as both  $D_1$  and  $D_2$  decrease.

**Table 7.7:** Possible Product Profiles for *STN-3 (Case-2.1)* Based on Mass Balance Only

CASE	MAIN-CUT-1			OFF-CUT-1			MAIN-CUT-2		
	$D_1$	$X^1_{D1}$	$X^2_{D1}$	$R_1$	$X^1_{R1}$	$X^2_{R1}$	$D_2$	$X^2_{D2}$	$X^3_{D2}$
A	2.01	0.950	<b>0.050</b>	<b>2.73</b>	<b>0.400</b>	0.600	5.26	<b>0.050</b>	0.950
B	1.98	0.950	<b>0.050</b>	<b>2.80</b>	<b>0.400</b>	0.600	5.22	<b>0.050</b>	0.950
C	1.89	0.950	<b>0.050</b>	<b>3.00</b>	<b>0.400</b>	0.600	5.11	<b>0.050</b>	0.950
D	1.68	0.950	<b>0.050</b>	<b>3.50</b>	<b>0.400</b>	0.600	4.82	<b>0.050</b>	0.950
F	1.60	0.950	<b>0.050</b>	<b>3.70</b>	<b>0.400</b>	0.600	4.70	<b>0.050</b>	0.950
G	1.58	0.950	<b>0.050</b>	<b>3.75</b>	<b>0.400</b>	0.600	4.67	<b>0.050</b>	0.950

## 7.6.2 Profit Calculations

The calculation procedure is described earlier. Using the product profiles of *Table 7.7* it was found that *Case-B* gives the maximum profit per batch. The results with cases *A* and *C* are presented in *Table 7.8*.

*Table 7.8* summarise the results as follows:

- Total number of batches per year  $N_B = 979.19$  in terms of fixed time = 7.67hr
- All the product quality is met on specifications
- The maximum profit achieved is with  $D_1 = 1.98$  kmol is 100746.7 \$/yr
- Off-cut 1 ( $R_1$ ) increases as both  $D_1$ ,  $D_2$  decrease.
- The product of  $R_1$  is not a desired product
- The net profit increase with increase the amount of main cuts-1 and 2.

The main cut products  $D_1$ ,  $D_2$  can affect the overall profitability (equation 7.1)

The number of plates for each column section was optimised together with vapour load to investigate how an optimal design would affect on overall profit Also the effect of off cut composition on design and operation is carried out (*Table 7.8*)

**Table 7.8:** Optimal Operation and Design for *STN-3 (Case-2.1)*

CASE	MAIN-CUT-1				OFF-CUT-1				MAIN-CUT-2			
	$D_1$	$X^1_{D_1}$	$X^2_{D_1}$	$X^3_{D_1}$	$R_1$	$X^1_{R_1}$	$X^2_{R_1}$	$X^3_{R_1}$	$D_2$	$X^1_{D_2}$	$X^2_{D_2}$	$X^3_{D_2}$
A	2.01	<b>0.950</b>	0.050	0.00	2.73	<b>0.397</b>	0.593	0.010	5.26	0.0	0.050	<b>0.950</b>
B	1.98	<b>0.950</b>	0.050	0.00	2.80	<b>0.395</b>	0.584	0.021	5.22	0.0	0.050	<b>0.950</b>
C	1.89	<b>0.950</b>	0.050	0.00	3.00	<b>0.400</b>	0.562	0.039	5.11	0.0	0.043	<b>0.957</b>

*PROFIT SUMMARY*

CASE	$CD_2$	$CD_3$	$CB_0$	$D_1$	$R_1$	$D_2$	$V$	$N$	$T$	$N_B$	$OC$	$CC$	$ACC$	$P$	$P$	$P$
	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	kmol/hr		hr	yr	\$/b	\$/b	\$/yr	\$/hr	\$/b	\$/yr
A	20.0	20.0	1.0	2.01	2.73	5.26	2.44	5, 5	7.67	979.1	0.45	32.42	31747.8	12.55	102.53	100395.7
B	20.0	20.0	1.0	<b>1.98</b>	3.80	<b>5.22</b>	<b>2.37</b>	<b>5, 4</b>	7.67	979.1	0.44	30.68	30038.4	12.60	102.90	<b>100746.7</b>
C	20.0	20.0	1.0	1.89	3.00	5.11	1.99	5, 4	7.67	979.1	0.37	27.71	27130.5	12.48	101.93	99806.3

## 7.7 Optimal Operation and Design with *STN-3*: (*Case Study-2.2*)

Referring to *STN-3* (*Figure 7.2*) ternary mixture with two main-cuts and one off-cut in between and following with the same procedure of that calculations (*Case study-2.1*) using the composition of (off-cut -1)  $x^1_{R1} = 0.10$  mole fraction to achieve the maximum profit. For this *STN*, the optimum product profiles and maximum profit achieved are presented in *Table 7.9*, and *Table 7.10*.

From *Table 7.9*, the following conclusions can be drawn:

1. The maximum possible value of  $D_2$  is shown 5.26 kmol, which is calculated based on the assumption that all of component 3 will be removed in main-cut 2.
2. The limits on the amount of products of this *STN* (*Figure 7.2*) could be summarised as follows:

$$(D_{1, \min}, D_{1, \max}) = (2.77, 2.97)$$

$$(R_{1, \min}, R_{1, \max}) = (1.76, 3.70)$$

$$(D_{2, \min}, D_{2, \max}) = (3.53, 5.26)$$

3. Off-cut 1 ( $R_1$ ) increases as both  $D_1$  and  $D_2$  decrease.

**Table 7.9:** Possible Product Profiles for *STN-3 (Case-2.2)* Based on Mass Balance Only

Case	Main-Cut-1			Off-Cut-1			Main-Cut-2		
	D1	X <sup>1</sup> <sub>D1</sub>	X <sup>2</sup> <sub>D1</sub>	R1	X <sup>1</sup> <sub>R1</sub>	X <sup>2</sup> <sub>R1</sub>	D3	X <sup>2</sup> <sub>D2</sub>	X <sup>3</sup> <sub>D2</sub>
A	2.97	0.950	<b>0.050</b>	<b>1.76</b>	<b>0.100</b>	0.900	5.26	<b>0.050</b>	0.950
B	2.95	0.950	<b>0.050</b>	<b>2.00</b>	<b>0.100</b>	0.900	5.05	<b>0.050</b>	0.950
C	2.89	0.950	<b>0.050</b>	<b>2.50</b>	<b>0.100</b>	0.900	4.61	<b>0.050</b>	0.950
D	2.84	0.950	<b>0.050</b>	<b>3.00</b>	<b>0.100</b>	0.900	4.16	<b>0.050</b>	0.950
E	2.79	0.950	<b>0.050</b>	<b>3.50</b>	<b>0.100</b>	0.900	3.71	<b>0.050</b>	0.950
F	2.77	0.950	<b>0.050</b>	<b>3.70</b>	<b>0.100</b>	0.900	3.53	<b>0.050</b>	0.950

### 7.7.1 Profit Calculations

The calculation procedure is described earlier. Using the product profiles of *Table 6.9* it was found that *Case-B* gives the maximum profit per batch. The results with cases *A* and *C* are presented in *Table 7.10*.

*Table 7.10* summarise the results as follows:

- Total number of batches per year  $N_B = 979.19$  in terms of fixed time = 7.67hr
- All the product quality is met on specifications
- The maximum profit achieved is with  $D_1 = 2.95$  kmol is 114570.0 \$/yr
- Off-cut 1 ( $R_1$ ) increases as both  $D_1$ ,  $D_2$  decrease.
- The product of  $R_1$  is not a desired product
- The net profit increase with increase the amount of main cuts-1 and 2.

The main cut products  $D_1$ ,  $D_2$  can affect the overall profitability (equation 7.1).

The number of plates for each column section was optimised together with vapour load to investigate how an optimal design would affect on overall profit Also the effect of off cut composition on design and operation is carried out (*Table 7.10*)

**Table 7.10:** Optimal Operation and Design for *STN-3* (Case-2.2)

CASE	MAIN- CUT-1					OFF- CUT-1			MAIN- CUT-2			
	$D_1$	$x^1_{D_1}$	$x^2_{D_1}$	$x^3_{D_1}$	$R_1$	$x^1_{R_1}$	$x^2_{R_1}$	$x^3_{R_1}$	$D_2$	$x^1_{D_2}$	$x^2_{D_2}$	$x^3_{D_2}$
A	2.97	<b>0.950</b>	0.049	0.001	1.76	<b>0.100</b>	0.890	0.009	5.26	0.0	0.050	<b>0.950</b>
B	2.95	<b>0.950</b>	0.042	0.008	2.00	<b>0.092</b>	0.806	0.102	5.05	0.0	0.050	<b>0.950</b>
C	2.89	<b>0.949</b>	0.041	0.010	2.50	<b>0.094</b>	0.659	0.247	4.61	0.0	0.050	<b>0.950</b>

<i>PROFIT SUMMARY</i>																
CASE	$CD_2$	$CD_3$	$CB_o$	$D_1$	$R_1$	$D_2$	$V$	$N$	$T,$	$N_B$	$OC$	$CC$	$ACC$	$P$	$P$	$P$
	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	kmol/hr		hr	yr	\$/b	\$/b	\$/yr	\$/hr	\$/b	\$/yr
A	20.0	20.0	1.0	2.97	1.76	5.26	2.64	8, 5	7.67	979.1	0.49	37.61	36824.4	14.26	116.5	114083.5
B	20.0	20.0	1.0	<b>2.95</b>	2.00	<b>5.05</b>	<b>1.85</b>	<b>12, 3</b>	7.67	979.1	0.34	32.66	31975.8	14.32	117.0	<b>114570.0</b>
C	20.0	20.0	1.0	2.89	2.50	4.61	1.74	<b>14, 2</b>	7.67	979.1	0.32	32.48	31799.8	13.12	107.2	104974.0

## 7.8 Optimal Operation and Design with *STN-3*: (Case Study-2.3)

Referring to *STN-3* in (Figure 7.2) ternary mixture with two main-cuts and one off-cut in between and following with same procedure of that calculations (Case study-2.1) with using the composition of (off-cut -1)  $x^1_{R1} = 0.050$  mole fraction to achieve the maximum profit.

For this *SNT*, the optimum product profiles and maximum profit achieved are presented in Table 7.11, and Table 7.12.

From Table 7.11, the following conclusions can be drawn:

1. The maximum possible value of  $D_2$  is shown 5.26 kmol, which is calculated based on the assumption that all of component 3 will be removed in main-cut 2.
2. The limits on the amount of products of this *STN* (Figure 7.2) could be summarised as follows:

$$(D_{1, \min}, D_{1, \max}) = (2.97, 3.07)$$

$$(R_{1, \min}, R_{1, \max}) = (1.67, 3.50)$$

$$(D_{3, \min}, D_{3, \max}) = (3.53, 5.26)$$

4. Off-cut 1 ( $R_1$ ) increases as both  $D_1$  and  $D_2$  decrease.

**Table 7.11:** Possible Product Profiles for *STN-3 (Case-2.3)* Based on Mass Balance Only

Case	Main-Cut-1			Off-Cut-1			Main-Cut-2		
	$D_1$	$X^1_{D_1}$	$X^2_{D_1}$	$R_1$	$X^1_{R_1}$	$X^2_{R_1}$	$D_3$	$X^2_{D_2}$	$X^3_{D_2}$
A	3.07	0.950	<b>0.050</b>	<b>1.67</b>	<b>0.050</b>	0.950	5.26	<b>0.050</b>	0.950
B	3.07	0.950	<b>0.050</b>	<b>1.75</b>	<b>0.050</b>	0.950	5.18	<b>0.050</b>	0.950
C	3.05	0.950	<b>0.050</b>	<b>2.00</b>	<b>0.050</b>	0.950	4.95	<b>0.050</b>	0.950
D	3.03	0.950	<b>0.050</b>	<b>2.50</b>	<b>0.050</b>	0.950	4.47	<b>0.050</b>	0.950
E	3.00	0.950	<b>0.050</b>	<b>3.00</b>	<b>0.050</b>	0.950	4.00	<b>0.050</b>	0.950
F	2.97	0.950	<b>0.050</b>	<b>3.50</b>	<b>0.050</b>	0.950	3.53	<b>0.050</b>	0.950

### 7.8.1 Profit Calculations

The calculation procedure is described earlier. Using the product profiles of *Table 7.11* it was found that *Case-A* gives the maximum profit per batch. The results with cases *B* and *C* are presented in *Table 7.12*

Note, slight discrepancies in composition  $D_2$  in both cases (*B* & *C*) takes place. *Table 7.12* summarise the results as follows:

The vapour load and number of trays in each column section were adjusted to achieve the desired purity specifications

- All the product quality is met on specifications
- The maximum profit achieved is with  $D_1 = 3.07$  kmol is 115697.7 \$/yr
- The net profit increase with increase the amount of main cuts-1 and main cut-2.

- Off-cut 1 ( $R_1$ ) increases as both  $D_1$ ,  $D_2$  decrease.
- The product of  $R_1$  is not a desired product
- The net profit increase with increase the amount of main cuts-1 and 2.

The main cut products  $D_1$ ,  $D_2$  can affect the overall profitability (equation 7.1). The number of trays for each column section was optimised together with vapour load to investigate how an optimal design would affect on overall profit Also the effect of off cut composition on design and operation is carried out (*Table 7.12*)

**Table 7.12:** Optimal Operation and Design for STN-3 (Case-2.3)

CASE	MAIN- CUT-1				OFF- CUT-1				MAIN- CUT-2			
	$D_1$	$X^1_{D_1}$	$X^2_{D_1}$	$X^3_{D_1}$	$R_1$	$X^1_{R_1}$	$X^2_{R_1}$	$X^3_{R_1}$	$D_2$	$X^1_{D_2}$	$X^2_{D_2}$	$X^3_{D_2}$
A	3.07	<b>0.950</b>	0.047	0.003	1.67	<b>0.052</b>	0.935	0.003	5.26	0.00	0.050	<b>0.950</b>
B	3.07	<b>0.950</b>	0.045	0.005	1.75	<b>0.046</b>	0.916	0.037	5.18	0.00	0.045	<b>0.954</b>
C	3.05	<b>0.950</b>	0.042	0.008	2.00	<b>0.050</b>	0.830	0.120	4.95	0.00	0.037	<b>0.962</b>

*P*

**PROFIT SUMMARY**

CASE	$CD_2$	$CD_3$	$CB_o$	$D_1$	$R_1$	$D_2$	$V$	$N_T$	$T$	$N_B$	$OC$	$CC$	$ACC$	$P$	$P$	$P$
	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	\$/kmol	kmol/hr		hr	yr	\$/b	\$/b	\$/yr	\$/hr	\$/b	\$/yr
A	20.0	20.0	1.0	<b>3.07</b>	1.67	<b>5.26</b>	<b>2.30</b>	<b>10,6</b>	7.67	979.1	0.42	38.02	37229.8	14.46	118.2	<b>115697.7</b>
B	20.0	20.0	1.0	3.07	1.75	5.18	2.18	11,5	7.67	979.1	0.40	36.89	36118.4	14.41	117.7	115264.0
C	20.0	20.0	1.0	3.05	2.00	4.95	1.96	13,3	7.67	979.1	0.36	34.73	34010.8	14.06	114.9	112515.3

## 7.9 Conclusions

In this State Task Network *STN-3*, the optimal set of design variable and operation of the Multivessel batch distillation column with two column sections for ternary mixture were presented by considering a comprehensive economic profit function that takes into account all design and operational cost trade-offs, instead of focusing a specific performance criteria such as batch time.

Purities of the main products are usually determined by market or downstream process requirements but the component recovery must be selected based on trade offs between distillation times, product values etc. Increasing the recovery of a particular species in a particular cut may have strong effects on the recovery of the other species in subsequent cuts or, in fact, on the ability to achieve at all the required purity specifications in the subsequent cuts.

Overall product demands, product quality and feed specifications allow calculation of product profiles (amount of each product) of each batch a priori using steady state mass balance calculations. Product profiles were generated based on fixing some of the variables such as amount of off cuts  $R$  and composition of off cuts  $x_R$ .

The composition of off cut -1  $x_{R1}^1$  is left as a decision variable in each case study. The effect of off cut compositions on the design and operation is carried out as shown in (Tables- 7.8, 7.10, 7.12).

Optimisation of design (number of trays and vapor load) is considered for ternary batch distillation in order to produce two main cuts with strict specifications, where the first main cut -1 is rich in component 1, and the last product is rich in the heaviest component-3 (main cut -2). The objective was to improve the profit function (\$/yr). For this *STN-2*, the optimal profit achieved was *Case-2.3 A* (117.7 \$/batch, and 115264.0 \$/yr), with optimum  $N = 16$  stages and  $V = 2.18$  kmol/hr, increases by 12.9% and 1.0 %, respectively, compared to the profits of other cases (*Case-2.1* and *Case-2.2*). This is due to the effect of off-cut compositions. Note, the overall profit increases with decrease of off-cut composition ( $x^1_{R1}$ ). The column to have high vapor loading and high number trays would increase capital cost and operating cost.

# CHAPTER 8

## CONCLUSIONS AND FUTURE RECOMMENDATIONS

### 8.1 Conclusions

#### 8.1.1 Process Modelling and Optimisation

Modelling and simulation of Multivessel batch distillation is discussed, the optimisation problems are also discussed briefly. The summary of the past work on optimisation of Multivessel batch distillation is reviewed.

gPROMS (**g**eneral **P**rocess **M**odelling **S**ystem) is a power general purpose modelling and optimisation environment, used to enhanced the design and operation of continuous and dynamic processes. There are several options within software, which allows developing different types of models; simple to rigorous. The gPROMS has been used for a wide variety of applications in petrochemicals, food, pharmaceutical, specialty chemical and automation. gPROMS has a number of advanced features including the ability to estimate an unlimited number of parameters and to use data from multiple steady-state and dynamic experiment. Its also gives the user complete flexibility in that, they can specify different variance model for different variables in different experiments. Moreover, it has a built-in interface to MS excel that allows the user to automatically test the statistical significance of results, generate plots overlaying model data and experimental data, plot confidence ellipsoids.

gPROMS has many advantages that make it an attractive tool for solving dynamic and steady state modelling problems and has been found to be easy, flexible, interactive and user-friendly software.

### **8.1.2 Operation and Design Optimisation**

In chapter five, for the first time, the optimisation problem is formulated to optimise the number of stages and vapor load for binary batch distillation under fixed product demand scenario for given product purity of mixture using *MultiVBD* column to maximise the overall profit, while the *CBD* column is evaluated against *MultiVBD* column for given separation task.

The profitability of *MultiVBD* was found to be significantly more profitable than in *CBD* column and it is demonstrated a reduction in energy consumption and the economical benefit becomes more apparent.

The dynamic optimisation problem is converted to nonlinear programming problem by Control Vector Parameterisation (CVP) technique and is solved by using efficient (SQP) method. The optimisation problem show that decreasing vapour load will decrease the operating cost (*OC*) and increase the profit *i.e.* vapour load showed very clear improvement in the annual profit.

### 8.1.3 Operation and Design Optimisation for Ternary Distillations

Based on a fixed product demand in terms of  $N$  and  $V$  of each product with strict product specifications, an optimal design and operation of ternary batch distillation was presented for both configurations (*CBD* and *MultiVBD*).

In chapter 6, two different profit functions are used, the first profit function is based on fixed operating cost (fixed design in terms of number of trays and vapour load) and exclude set-up time and capital cost ( $CC$ ). The appropriate comparison could not be made between two configuration columns due to fixed design.

The second profit function is based on variable design in terms of number of trays, vapour load, operating cost and annulised capital cost. Again, the appropriate comparison is made between *MultiVBD* and *CBD*, it was found that the profitable of *MultiVBD* column is more than that in *CBD* column.

### 8.1.4 Operation and Design Optimisation of Multivessel Batch Column

Two State Task Networks (*STNs*) different to that presented in chapter 6 are considered for *MultiVBD* column only.

The first *STN* -2 is with two off-cuts and two main cuts to be produced for given product specifications. The second *STN* -3 is with two main-cuts and one off-cut. The objective is to maximise the overall profit with desired purities in terms of key component mole fraction ( $x^1_{D1}$ ,  $x^2_{D2}$ , and  $x^3_{D2}$ ). Product profiles were generated based on fixing of some of the

variables such as amount of off-cut and its composition. The optimal design in terms of vapour load and number of trays together are optimised to achieve the required specifications for main-cuts.

In this chapter, the optimal design and operation of *MultiVBD* column is considered under strict product quality specifications. Overall product demands, product quality and feed specifications allow calculation of product profiles (amount of each product) of each batch using steady state mass balance calculations. In all cases, product demand and quality are met on specifications.

## **8.2 Future Recommendations**

Here are the recommendations which are to follow this study:

- The optimal design and operation policies in batch distillation under fixed product demand and strict product specifications was presented with only simple dynamic model, the rigorous dynamic model could be considered and compared with these results.
- Different scenarios of main-cut/off-cut products (with and an off-cut recycle), and dealing with off-cut production, and treat any over or under production for *MultiVBD* column could be considered to achieve maximum total profit and evaluated against the performance of Conventional batch distillation column *CBD*.

- Effect of factors such as different feed compositions and product specifications on the column specification and operation on the *MultiVBD* could be considered.

The overall purpose of the future work will be providing a better understanding of the optimal design and operation of Multivessel batch column, especially; to show how the optimal design (in terms of column specification), and optimal recovery of product with off-cut recycling under fixed demand is effected on the overall profitability, and highlight the effects of factors such as feed composition and product specification on the optimal design and operation on the system

## REFERENCE

Abrams, H.J., Miladi, M.M. and Attarwala, T.F., **1987**, “Preferable alternatives to Conventional Batch Distillation”. *Distillation and Absorption 1987, I. Chem. E. Symposium Series No. 104*, Brighton, UK, 7-9 September.

Attarwala, F.T. and Abrams, H.J., **1974**, “Optimisation Techniques in Binary Batch Distillation”, *IChemE Annual Research Meeting, London*.

Al-Tuwaim, S.M and Luyben, W.L., **1991** “Multicomponent batch distillation. 3. Shortcut design of batch distillation columns”, *Ind. Engineering Chemical research*, **30**, pp 507-516.

Barolo, M., Guarise, N., Rienzi, S.A., Trotta, A., and Macchietto, S., **1996 b** “Running Batch Distillation in a Column with a Middle Vessel”, *Ind. Eng. Chem. Res.*, **35**, pp. 4612–4618.

Barolo, M., Guarise, G.B., Rienzi, S.A., and Trotta, A., **1998** “Understanding the Dynamic of Batch Distillation Column with a Middle Vessel” *Computers and Chem. Eng.*, **22**, ppS37-S44

Bernot, C., Doherty, M.F and Malone, M.F., **1991** “Design and operating policies for multicomponent batch distillation”, *AIChE* **32**, pp 293-301.

Bonny, L., **2006**, “Multicomponent Batch Distillations Campaign: Control Variable and Optimal Recycling Policy”, *Ind. Eng. Chem. Res.*, **45**,(26) pp.8998-9009.

Bortolini, P. and Guarise, GB., **1970** “A new Practice of Batch Distillation (in Italian)”, *Quad. Ing. Chim. Ital.*, **6**, (9) pp.150-159.

Boston, J.F., Britt, H.I., Jirapongphan, S. and Shah, V.B., **1980**, “An Advanced System for the Simulation of Batch Distillation Operation”, *In Foundation of Computer Aided Chemical Process Design*, New York, II, pp.203-237

Chen, C.L., BP Research, Sunbury, UK Private communication, **1995**.

Christensen, A.C., Jorgensen, E.W., Perkins, J.D. and Skogestad, S., **1979**, “On the dynamics of batch distillation: a study of parametric sensitivity in ideal binary columns” Presented at the AIChE Annual Meeting, Miami, USA, November, paper no.184d.

Christensen, F.M. and Jorgensen, S.B., **1987** “Optimal control of binary distillation with recycled waste cut”, *Chem. Eng. J.*, **34**, pp.57-64

Distefano, G.P., **1968**, “Mathematical Modelling and Numerical Integration of Multicomponent Batch Distillation Equation”, *AICHE J.*, **14** (1) pp.190-199.

Coward, I., **1967**, “The time optimal problem in binary batch distillation”, *Chem.Engng.Sci.*, **22** (4), pp.503-5116.

Diwekar, U.M. and Madhavan, K.P., **1986**, “Optimal design of multicomponent batch Distillation Column”, *Proceedings of World Congress III of Chemical Engineering*, Sept., Tokyo, **4**, pp.719.

Diwekar, U.M., Madhavan, K.P., and Malik, R.K., **1987**, “Optimal reflux rate policy determination for multicomponent batch distillation columns”, *Comput. Chem. Engng.*, **11**, pp.629.

Diwekar, U.M., Madhavan, K.P., and Swaney, R.E., **1989**, “Optimisation of multicomponent batch distillation columns”, *IEC.Res.*, **28**, pp.1011-1017.

Diwekar, U.M. and Madhavan, K.P., **1991**, “Multicomponent batch distillation column design”, *IEC.Res.*, **30**, pp.713-721.

Diwekar, U.M., **1992**, “Unified approach to solving optimal design-control in batch distillation columns”, *AIChE J.*, **38** (10), pp.1551-1563.

Diwekar, U.M., **1995** “Batch distillation: Simulation, Optimal Design and Control”, Taylor and Francis, Washington, D.C.

Domenech, S and Enjalbert, M., **1981**, “Program for Simulation Batch Rectification as a unit operation”, *Comput.Chem.Engng.* **5** (3), pp.181-185.

Eykhof, **1974**, System Identification, J. Wiley, London.

Fetisov, Yu. M., Efremov, A.A, Falin, V.A., Egurnov, V. Ya. and Zel'venskii, Ya.d., **1977**, "Calculation of Design Parameters of the Periodic Fractionation of Dilute Solutions (in Russian)", *Tr. Mosk. Khim. Tekhnol. inst.*, **96**, pp.62.

Franks, O.R., **1972**, "Modelling and Simulation in Chemical Engineering", *John Wiley and Sons*, New York.

Farhat. S., Czernicki, M., Pilbouleau, L. and Domenech, S., **1990**, "Optimisation of multiple-fraction batch distillation by linear programming", *AIChE J.*, **36** (9), pp.1349-1360.

Furlonge, H.I., Pantelides, C.C. and Sorensen, E., **1999**, "Optimal Operation of Multivessel Batch Distillation", *AIChE J.* **45** (4), pp.781-801.

Furlonge, H.I., **2000**, "Optimal Operation of Unconventional Batch Distillation Columns", PhD Thesis, University of London.

Galindez, H and Fredenslund, A., **1988**, "Simulation of Multicomponent Batch Distillation Processes", *Comput. Chem. Engng.*, **12** (4), pp.281-288.

Gary, J.H. and Handwerk, G.E. **1984**, *Petroleum Refining technology and Economics* (2<sup>nd</sup> ed.) Marcel Dekker, Inc.

Gear, C.W., **1971** "Simultaneous numerical solution of differential-algebraic equation", *IEEE Trans. Circuit Theory* **CT-18** (1), pp.89-95.

Gonzalez-Velasco, J.R., Gutierrez-Ortiz, M.A., Castresana-Pelayo, J.M and Gonzalez-Marcos, J.A., **1990**, “Modelling of Batch Distillation by Pulse Response Method”, *Int. Chem. Eng.*, **30** (3), pp.568-576.

Greaves, M A., Mujtaba, I.M., Barolo, M., Trotta, A. and Hussain, M.A., **2003**, “Neural Network Approach to Optimisation of Batch Distillation – Application to a Middle vessel Column” *Trans. IChemE, Part A*, **81** (3), pp.393-401.

Hansen, T.T and Jorgensen, S.B, **1986**, “Optimal control of binary batch distillation in tray or packed columns” *Chem. Eng. J.*, **33**, pp.151-155.

Hasebe, S., Abdul Aziz, B.B., Hashimoto, I. and Watanabe, T., **1992**, “Optimal Design and Operation of Complex Batch Distillation Column”, *In Proceedings IFAC Workshop*, London, 7-8 September, p.177.

Hasebe, S., Kurooka, T., and Hashimoto, I., **1995**, “Comparison of the Separation Performances of a Multi-Effect Batch Distillation System and a Continuous Distillation System” *Symposium DYCORD*, helsiger- Denmark, June, 7-9 pp.249-254.

Hasebe, S., Noda, M., Hashimoto, I., **1999**, “Optimal Operation for Total Reflux and Multi-Effect Batch Distillation System,” *Comput. Chem. Eng.*, **23**, pp.523-532.

Hindmarsh, A.C., 1980, “LSODE and LSODI, two new initial value ordinary differential equation solvers”, *Ass.Comput.Mach., Signam Newsl.*, **15** (4), pp.10-11

Holland, C.D. and Liapis, A.I., **1983**, “Computer Methods for Solving Dynamic Separation Problems”, *McGraw-Hill Book Company*, New York, USA.

Huckaba, C.D. and Danly, D.E., **1960**, “Calculation procedures for binary batch rectification”, *AIChE J.*, **6**(2), pp.335-342.

Kondili, E., Pantelides, C.C. and Sargent, R.W.H. In Proceedings of 3rd *International Symposium on Process Systems Engineering*, (1988) 62.

Jenkins, M.J., Coalite Chemicals, **2000**, UK. *Private communication*.

Lang, .C.A. **1995** “The Possibility of a Cyclic Mechanism for Acid-Cataysed Ester Hydrolysis” *J. Am. Chem.*, **86**, pp.2521-2523

Li, P., Hoo, H.P. and Wozny, G., **1998** “Efficient simulation of batch distillation process by using orthogonal collection”, *Chem.Eng.Technol.*, **21** (11), pp.853-862.

Lloyd, L.E., **1950**, “Batch Distillation Characteristics and Limitations of Batch Still”, *Pet. Refiner*, **29**(2),pp.135.

Logsdon, J.S., and Biegler, L.T., **1993** “Accurate determination of optimal reflux policies for the maximum distillate problem in batch distillation” *IEC Res.*, **32** (4), pp.692-700.

Logsdon, J.S., Diwekar, U.M. and Biegler, L.T., **1990**, “ On The Simultaneous Optimal Design and Operation of Batch Distillation, *Trans.IChemE*, 68A pp.434.

Low, K.H.and Sorensen, E., **2003**, “Simultaneous Optimal Design and Operation of Multivessel Batch Distillation”, *AIChE J.*, 49, pp.2564-2576

Low, K.H.and Sorensen, E., **2004**, “Simultaneous Optimal Design and Operation of Multipurpose Batch Distillation Columns”, *Chem. Eng. Prog.* **43** (3), pp.273-289.

Low, K.H. and. Sorensen, E., **2005**, “Simultaneous optimal configuration, design and operation of batch distillation”, *AIChE J*, **51** (6), pp.1700-1713.

Lucet, M., Charamel, A., Champuis, A Guido, D. and Loreau, J., **1992**, “Role of batch processing in the chemical process industry”, *In Proceeding of NATO ASI on Batch Processing Systems Engineering*, Antalya, Turkey, May 29-June 7

Luiz, A. V and Ruiz, J M, **2006**, “Optimal Programming of Batch Distillation: Vessel Network Operation” *Latin American Applied Research*, **36**, pp.221- 228.

Luyben, W.L., **1988** “Multicomponent Batch Distillation. 1 Ternary system with slop recycles”, *IEC Res.*27, pp.642-648.

Mahmud, M. T., Mujtaba, I. M., Emtir, M., **2008** “Optimal Design and Operation of multivessel Batch Distillation Column with Fixed Product Demand and Strict Product Specifications, *Comput. Aided Chem. Eng.*, **25**, pp.859-864.

Mayur, D.N. and Jackson, R. **1971**, “Time-optimal Problems in batch Distillation for Multicomponent Mixtures and for Columns with holdup”, *Chem. Eng. J.*, **2**, pp.150.

Meadow, E.L., **1963**, “Multicomponent Batch Distillation Calculations on a Digital Computer”, *Chem. Eng. Prog. Symp. Ser.*, **59** (46), pp.48-60

Miladi, M.M and Mujtaba, I.M., **2004**, “Optimisation of Design and Operation Policies of Binary Batch Distillation with Fixed Product Demand” *Computers and Chem. Eng.*, **28**, pp.2377-2390.

Miladi, M.M and Mujtaba, I.M., **2005**, “The Effect of Off-Cut recycle on the Optimum Design and Operation of Binary Batch Distillation with Fixed Product Demand”, *Computers and Chem. Eng.*, **29**, pp.1687-1695.

Miladi, M.M and Mujtaba, I.M., **2006**, “Optimisation of Design and Operation Parameters for Ternary Batch Distillation with Fixed Product Demand”, *Eng. Computations: International Journal*, **23**, (7), pp.771-793.

Mori, H., Goto, H., Yang, Z.C., Aragaki, T and Koh, S., **1995**, “A stagewise a logarithm for multicomponent multistage batch distillation calculation”, *J Chem. Eng. Japan.*, **28**, pp.576-588.

Mujtaba I.M. and Macchietto, S., **1992** “An Optimal Recycle Policy for Multicomponent Batch Distillation” *Computers and Chem. Eng.*, **16S**, pp.S273-S280.

Mujtaba I.M. and Macchietto, S., **1993**, “Optimal Operation of Multicomponent Batch Distillation Multiperiod Formulation and Solution”, *Comput. Chem. Engng.*, **17** (12),pp. 1191-1207

Mujtaba I.M. and Macchietto, S., **1994** “Optimal Operation of Multicomponent Batch a Comparative Study Using Conventional and Unconventional Columns”, In Proceedings *ADCHEM' 94-IFAC Symposium on Advanced Control of Chemical Processes*, Kyoto, Japan, 25-27 May, pp.401-406.

Mujtaba I.M. and Macchietto, S., **1996**, “Simultaneous Optimisation of Design and Operation of Multicomponent Batch Distillation Column-Single and Multiple Separation Duties”, *J. Proc. Cont.*, **6** (1), pp.27-36

Mujtaba I.M., **1997**, “Use of Continuous Distillation Columns for Batch Separation”, *Trans.IChemE.*, **75** Part A, September, (24),pp.609-619

Mujtaba I.M. and Macchietto, S., **1998**, “Holdup Issues in Batch Distillation Binary Mixtures” *Chem. Eng. Sci.*, **53** (14), pp.2519-2530.

Mujtaba, I.M., **2004**,”Batch Distillation: Design and Operation”, Imperial College Press, London, UK.

Naphtali, L.M. and Sandholm, D.P., 1971, “Multicomponent separation calculations by linearisation” *AICHE. J.*, **17** (1), pp.148-160

Noda, M., Chida, T., Hasebe, S., and Hashimoto, I., **2000**, “On-Line Optimisation System of Pilot Scale Multi-Effect Batch Distillation System”, *Comput. Chem. Eng.*, **24**, pp.1557-1583

Parakrama, R., **1985**, *The chemical Engineer*. September, 24.

Perkins J. And Walsh S. **1996**, “Optimisation as a Tool for Design/Control Integration” *Comput. Chem. Eng.*, **20**, (4) pp.315-323.

Rayleigh, J.W.S., **1902**, “On the Distillation of Binary Mixture”, *Phil. Mag.*, 6<sup>th</sup>. Series, **4** (23), pp.521-527.

Rippin, D.W., 1983, “Simulation of single- and multiproduct batch chemical plants for optimal design and operation”, *Comput. chem. Engng.* **7** (3), pp.137-165.

Robinson, E.R., **1969**, “The optimisation of batch distillation operations”, *Chem.Engng.Sci.*, **42**(11), pp.1661-1668.

Robinson, E.R., **1970**, “The optimal control of an industrial batch distillation column”, *Chem.Engng.Sci.*, **25**(6), pp.921-930.

Robinson, C.S., and E. R. Gilliland, **1950**, *Elements of fractional distillation*, 4th ed., *McGraw-hill*, NY.

Rose, A., William, T.J. and Prevost, C., **1950**, “Holdup in Batch Distillation Critical Reflux Ratio”, *Ind. Eng. Chem.*, **42** (10), pp.1876-1879.

Ruiz, C.A., **1988**, “A generalised dynamic model applied to multicomponent batch distillation. Proceedings *CHEMDATA* 88, 13-15 June, Sweden, pp.330-340.

Safrit, B.T. and A.W. Westerberg, **1994**, *IEC Res.*36, p.436.

Skogestad, S., Wittgens, B., Litto, R. and Sorensen E., **1997**, “Multivessel Batch Distillation”, *AIChE J.* **43**, pp 971-978.

SimiSci, **1997**, Simulation Sciences Inc. USA.

Sorensen, E. and S. Skogestad (**1996**), “Comparison of inverted and regular batch distillation”, *Chem. Eng. Sci.*, **51**(22), pp.4949-4962.

Stewart, R.R., Weisman, E., Goodwin, B.M. and Speight, C.E., **1973**, “Effect of Design Parameters in Multicomponent Batch Distillation”, *Ind. Eng. Chem. Process. Des. Development*, **12** (2), pp.130-136

Sundaram, S. and Evans, L.B., **1993a** “A Short-Cut Procedure for Simulating Batch Distillation Operations”, *IEC Res*, **32**, pp.500-510.

Sundaram, S. and Evans, L.B., **1993b** “Synthesis of separations by batch distillation” *IEC Res.*, **32**, pp511-518.

Teresa, M.M and Calos, A.V., **2003**, "Computer Modelling and Simulation Chemical Processes Pollution Prevention", Coimbra. July 4.

Winkel, M.L., Zullo, L.C., Verheijen, P.J., and Pantelides, C.C., **1995**, "Modelling and Simulation of the Operation of an Industrial Batch Plant using gPROMS", *Computers and Chem. Eng.* **19**, pp.571-576.

Wittgens, B., R Litto, E. Sorensen, and S. Skogestad, **1996**, "Total Reflux Operation of Multivessel Batch Distillation", *Computers and Chem. Eng.*, **S20**, pp.S1041-S1046.

Wittgens, B., and S. Skogestad, **2000**, "Closed Operation of Multivessel Batch Distillation: Experimental Verification," *AIChE J.* **46**, pp.1209-1221.

Young, H.K, **1999** "Optimal Design and Operation of a Multi-product Batch Distillation Column Using Dynamic Model", *Chem. Eng. and Processing*, **38**, pp.61-72.

Zamprogna, E., Barolo, M. and Seborg, D.E **2001**, "Composition Estimation in a Middle Vessel Batch Distillation Column Using Artificial Neural Networks", *Trans. IChemE*, **79A**, Pt. A, pp.689-696.

# APPENDIX

## **gPROMS Computer Program for Solving Strict Product Specifications problems for Simple Model for Multivessel Batch Distillation Column.**

This system consists of 3 column sections, 2 intermediate vessel, reboiler, total condenser and accumulator (trays are numbered from the top and down). Vapour bypassing the intermediate vessels.

There are 3 components, the lightest product is accumulated in the condenser, the second lightest in the upper vessel, the third lightest in the lower vessel and the heaviest in the reboiler.

The mathematical model assumes constant relative volatility (relative to the heaviest component).

### **Model File**

#### **PARAMETER**

NoComp

nt           As     Integer

nm           As     Integer

nb           As     Integer

## VARIABLE

RelVolatility As Array (NoComp) of NoType

Vapor load As VaporBoilupRate

### # holdup

H\_condenser As MolarHoldup # kmol

H\_reboiler As MolarHoldup # kmol

H\_plate As MolarHoldup # kmol

H\_feedtank As MolarHoldup # kmol

H\_feedtank2 As MolarHoldup # kmol

### # liquid rate

LiqRate As LiquidFlowrate # kmol/hr 1

liqrte\_feed As LiquidFlowrate# kmol/hr

liqrte\_f As LiquidFlowrate# kmol/hr

### # liquid composition

x\_tankfeed As Array (NoComp) of MolarFraction

x\_tankfeed2 As Array (NoComp) of MolarFraction

x\_condenser As Array (NoComp) of MolarFraction

x\_reboiler As Array (NoComp) of MolarFraction

x\_plate As Array (nb,NoComp) of MolarFraction

y\_reboiler As Array (NoComp) of MolarFraction

y\_plate As Array (nb,NoComp) of MolarFraction

## EQUATION

### # Material balance for condenser

$$V_{load} = LiqRate;$$

$$H_{condenser} = V_{load} - LiqRate;$$

$$x_{condenser} = (V_{load}/H_{condenser}) * (y_{plate(1)} - x_{condenser});$$

### # Material balance for trays

$$x_{plate(1)} = (1/H_{plate}) * (LiqRate * (x_{condenser} - x_{plate(1)})$$

$$+ V_{load} * (y_{plate(2)} - y_{plate(1)}));$$

### # Phase equilibrium

$$y_{plate(1)} = RelVolatility * x_{plate(1)} / \text{Sigma}(RelVolatility * x_{plate(1)});$$

#### for j: = 2 to nt-1 do

$$x_{plate(j)} = (1/H_{plate}) * (LiqRate * (x_{plate(j-1)} - x_{plate(j)})$$

$$+ V_{load} * (y_{plate(j+1)} - y_{plate(j)}));$$

### # Phase equilibrium

$$y_{plate(j)} = RelVolatility * x_{plate(j)} / \text{Sigma}(RelVolatility * x_{plate(j)});$$

#### END

$$x_{plate(nt)} = (1/H_{plate}) * (LiqRate * (x_{plate(nt-1)} - x_{plate(nt)})$$

$$+ V_{load} * (y_{plate(nt+1)} - y_{plate(nt)}));$$

### # Phase equilibrium

$$y_{plate(nt)} = RelVolatility * x_{plate(nt)} / \text{Sigma}(RelVolatility * x_{plate(nt)});$$

### # Material balance for the vessels

$$H_{feedtank} = liqrate - liqrate_{feed};$$

$$H_{feedtank2} = liqrate_{feed} - liqrate_f;$$

```

$x_tankfeed = (1/H_feedtank) *(liqrte*x_plate (nt,)-liqrte_feed*x_tankfeed);
$x_tankfeed2 = (1/H_feedtank2)*(liqrte_feed*x_plate (nm,)-
liqrte_f*x_tankfeed2);
$x_plate (nt+1,) = (1/H_plate) * (liqrte_feed* (x_tankfeed-x_plate (nt+1,)) +
vload* (y_plate (nt+2,) - y_plate (nt+1,)));
y_plate (nt+1,) = RelVolatility*x_plate (nt+1,) / Sigma (RelVolatility* x_plate
(nt+1,));

```

**for j: = nt+2 to nm-1 do**

```

$x_plate (j,) = (1/H_plate)*(liqrte_feed*(x_plate (j-1,)-x_plate (j,))
+vload*(y_plate (j+1,)-y_plate (j,)));
y_plate (j,) = RelVolatility*x_plate (j,) / Sigma (RelVolatility*x_plate (j,));

```

**END**

```

$x_plate (nm,) = (1/H_plate)*(liqrte_feed*(x_plate (nm-1,)-x_plate (nm,))
+ Vload*(y_plate (nm+1,)-y_plate (nm,)));
y_plate (nm,) = RelVolatility*x_plate (nm,) / Sigma (RelVolatility*x_plate (nm,));

```

**# Feed tank**

```

$x_plate(nm+1,)=(1/H_plate)*(liqrte_f*(x_tankfeed2-
x_plate(nm+1,))+vload*(y_plate (nm+2,)-y_plate(nm+1,)));
y_plate(nm+1,) = RelVolatility*x_plate(nm+1,) / Sigma (RelVolatility*
x_plate(nm+1,));

```

**for j := nm+2 to nb-1 do**

```

$x_plate(j,)=(1/H_plate)*(liqrte_f*(x_plate(j-1,)-x_plate(j,))+vload*(y_plate(j+1,)-
y_plate(j,)));
y_plate(j,) = RelVolatility*x_plate(j,) / Sigma (RelVolatility*x_plate(j,));

```

**END**

```

$X_plate(nb,)=(1/H_plate)*(liqrte_f*(x_plate(nb-1,)-
x_plate(nb,))+vload*(y_reboiler -y_plate(nb,)));
y_plate(nb,) = RelVolatility*x_plate(nb,) / Sigma (RelVolatility*x_plate(nb,));

```

### **# Reboiler**

```

$H_reboiler = liqrte_f- Vload ;
$X_reboiler=(1/H_reboiler)*(liqrte_f*(x_plate(nb,)-x_reboiler)-vload*(y_reboiler-
x_reboiler));
y_reboiler = RelVolatility*x_reboiler / Sigma (RelVolatility*x_reboiler);

```

### **Process File**

#### **UNIT**

mtvbd as mvbd

#### **SET**

WITHIN mtvbd DO

#### **# SECTION -1 (TOP)**

nt:=4;

#### **# SECTION -2 (MIDDEL)**

nm:=10;

#### **# SECTION -3 (Bottom)**

nb:=14;

# No of component

NoComp:=3;

#### **END**

## ASSIGN

WITHIN mtvbd DO

vload : =2.3; # kmol/hr

liqrate\_feed =2.3; # kmol/hr

H\_plate: =0.012; # kmol

liqrate\_f: = 6; # kmol/hr

RelVolatility: =[8,4,1];

## END

## INITIAL

WITHIN mtvbd DO

### # X-CONDENSER

H\_condenser = 2.61;

x\_condenser(1) = 0.30;

x\_condenser(2) = 0.20;

x\_condenser(3) = 0.50;

### # X-PLATES

x\_plate (,1) = 0.30;

x\_plate (,2) = 0.20;

x\_plate (,3) = 0.50;

### # X\_TANK FEEDS

H\_feedtank = 0.83; # kmol

x\_tankfeed(1) = 0.30;

x\_tankfeed(2) = 0.20;

x\_tankfeed(3) = 0.50;

## # X\_TANK FEEDS2

H\_feedtank2 = 1.24; # kmol  
x\_tankfeed2(1) = 0.30;  
x\_tankfeed2(2) = 0.20;  
x\_tankfeed2(3) = 0.50;

## # X\_REBOILER

H\_reboiler = 5.32; # kmol  
x\_reboiler(1) = 0.30;  
x\_reboiler(2) = 0.20;  
x\_reboiler(3) = 0.50;

**END**

## **SOLUTION PARAMETERS**

g excel output := on;  
DASolver := "SRADAU" [  
"OutputLevel" := 0,  
"InitialisationNLSolver" := "NLSOL" [  
"OutputLevel" := 0, ],  
"ReinitialisationNLSolver" := "NLSOL" [  
"ConvergenceTolerance" := 1e-005,  
"EffectiveZero" := 1e-005,  
"FDPerturbation" := 1e-005,  
"MaxFuncs" := 1000000,  
"MaxIterNoImprove" := 100,  
"MaxIterations" := 1000,

```

"NSStepReductions" := 10,

"OutputLevel" := 0,

"SLRFactor" := 50,

"SingPertFactor" := 0.01,

"UseBlockDecomposition" := TRUE,

"LASolver" := "MA48"],

        ]; # "DASOLV";}

{ NLSolver := "BDNLSOL" [ "BlockSolver" := "SPARSE" [

"ConvergenceTolerance" := 1e-006]];

DOSolver := "CVP_SS" ["OutputLevel" := 0;

"MINLPSolver" := "SRQPD" [

"OutputLevel" := 0;

"MinimumLineSearchStepLength" := 1e-05;

"OptimisationTolerance" := 0.001]

        ];}

ReportingInterval := 0.01 ;

SCHEDULE

```

**Continue for 7.67 # hr**