Modeling of Crude Distillation Unit

by

Nasibah Hartono

Dissertation submitted in partial fulfilment of

the requirements for the

Bachelor of Engineering (Hons)

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Universiti Teknologi PETRONAS

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CERTIFICATION OF APPROVAL

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Approved by,

AP. Dr. Marappagounder Ramasamy
Project Supervisor

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

July 2010

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

NASIBAH HARTONO

ABSTRACT

Modeling of CDU is today the foundation to almost any operation including design, control, planning and retrofitting of the refinery plant. The purpose of this project is to develop Rigorous model of Crude Distillation Unit (CDU) and also to study the dynamic behavior of the model. In other to develop more accurate model, linearized Francis Weir formula is selected to model liquid flow dynamic. Beside Francis Weir, two different assumptions are studied to improve the model, which are constant molar flow and non-constant flow. In constant molar flow model, the column is assumed to be constant pressure so the vapor flow for each stage is the same and therefore the energy equations is neglected. Since the dynamic model can be subjected to disturbance and used for over a wide pressure, the assumption is not accurate and therefore non constant molar flow assumption is important. The scope of work in this project is firstly to perform Rigorous modeling for CDU where mass, energy balance, equilibrium relation and Francis Weir formula where all the equations are developed. Then, in other to get input properties for the model, process modeling simulator, ASPEN HYSYS is used to simulate CDU. The famous computer algebra, MATLAB is used to solve the dynamic rigorous model simultaneously. Lastly, the results of the model dynamic behavior will be studied. In this report, only constant molar flow model is solved and discussed where non constant molar flow is only discussed in Literature Review and Methodology due to its complexity and also time constrain.

This report consists of 5 main chapters; the 1st chapter which is Introduction briefly explains the problem statement, objectives of research, the scope works and work flow of FYP 1 and also the Gantt chart. The 2nd chapter which is Literature Review covers the background of Crude Distillation Unit (CDU) and also the theory of distillation to model the CDU. The 3rd chapter which is Methodology will explain the steps on how to develop mathematical modeling, how to determine the inputs from HYSYS and also how to do MATLAB computational. The 4th chapter is Results and Discussion which all the results from MATLAB computational is shown and analyzed. The last chapter consists of Conclusion and Future Recommendation.

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Firstly, my sincere and grateful thanks to my supervisor, AP.Dr.M. Ramasamy for his informative supervision and countless hours spent in sharing understanding, profound knowledge and valuable experiences throughout the project. I appreciate all his effort in providing advice, great support and assistance that enable this project to achieve its objectives and be completed successfully within the time frame given.

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Last but not least, special credit goes to my parents, family members, Final Year Project committee, colleagues, and friends, who had dedicatedly provided me with additional support and encouragement throughout this project. Thanks again to all, your kindness and helps will always be remembered.

LIST OF FIGURES

Figure 4.2(d): Simulated responses in distillate composition versus time for +10% step change in F

Figure 4.2 (e): Simulated Responses in Reboiler Composition versus time for +10% step change in F

Figure 4.2(f): Simulated Responses in Reboiler Holdup versus time for +10% step change in F (MB vs t)

LIST OF TABLES

TABLE OF CONTENTS

NOMENCLATURE

B	Reflux
D	Boilup
$H_{i,j}$	Vapor enthalpy for *i*th component on *j*th stage
$h_{i,j}$	Liquid enthalpy for *i*th component on *j*th stage
$h_{fi,j}$	Feed enthalpy of *i*th component in the feed to *j*th stage
h_{ow}	Height of liquid over weir
$K_{i,j}$	Phase equilibrium constant of *i*th component on *j*th stage
L_j	Total liquid flow rate from *j*th stage
L_{ij}	Liquid flow rate of *i*th component from *j*th stage
l_w	Length of weir
M_j	Total liquid holdup on jth tray
N_T	Total number of stages in the column (at Condenser Stage)
N_C	Total number of pseudo-components in the feed
N_F	Feed Stage
N_P	Side Product Stage
p_i°	Vapor pressure of ith component
p_i^c	Critical pressure of ith component
q	Feed Liquid Fraction
Q_j	Heat duty of the *j*th stage
$T_{avg,i}$	Mean average boiling point of *i*th pseudo-component
T_j	Temperature of *j*th stage
T_r	Reduced Temperature
V_j	Total vapor flow rate from the *j*th stage
$v_{i,j}$	Vapor flow rate of *i*th component from *j*th stage
w_j^l	Liquid side stream from stage *j*th
w_i	Acentric factor of ith component
w_j^v	Vapor side stream of from *j*th stage
$x_{i,j}$	Mole fraction of *i*th component in liquid phase on *j*th stage
$y_{i,j}$	Mole fraction of *i*th component in vapor phase on *j*th stage
$z_{i,j}$	Mole fraction of feed on *j*th stage

CHAPTER 1
INTRODUCTION

1.1 Background and Significant of Project.

The crude distillation unit (CDU) is one of the most important refinery operations fractionating preheated crude oil into respective product fractions like Heavy Naphtha HN, Kerosene SK, Aviation Turbine Fuel ATF, Light Gas Oil LGO, Heavy Gas Oil HGO, Reduced Crude Oil RCO and etc. Therefore, it becomes extremely important to model the crude distillation unit to predict the composition of products from various crudes, which are processed under different operating condition. The model thereby acts as an essential tool for production planning and scheduling, economic optimization and real-time online control and performance optimization. Additionally, such a model is also an essential prerequisite for a project engineer attempting either design of new units or rating of existing units [4].

1.2 Problem Statement

Modeling and simulation of distillation columns are not a brand new research area. Several papers during the last two decades have been written on the modeling and simulation of distillation columns. Most of these models are based on a set of simplifications and have been used for the simple applications depending on the nature of assumptions ((Gani et al. (1986) and Choe and Luyben (1987)) [3]. Among the examples of simplification are no flow dynamic (constant hold up) and the assumption of constant pressures of all trays (constant molar flow), which is often justified because of tight pressure control. As stated by Choe and Luyben (1987), constant molar flow may be valid for moderate to high pressure columns when the relative changes in pressure are very small. They show that for vacuum columns, these assumptions lead to significant errors in time constants, temperatures and flow rates Obviously, dynamic models used for over a wide pressure, e.g. during startup and shutdown simulations; such an assumption cannot be used. In Wittgens and Skogestad's research (1995), more complex model results in a better agreement with experimental data as compared with a simpler one which is based on no flow dynamics and constant molar flows by neglecting the energy balance equation [7].

Therefore, in order to achieve more accurate model of dynamic CDU, this research focuses on the development of a Rigorous model for dynamic distillation column considering the material and energy balances, equilibrium relations and the dynamic flow on each tray.

1.3 Objectives of Research

The purposes of this research are:

- To develop a more accurate Rigorous model of dynamic crude distillation unit by considering flow dynamic. This model is solved by using MATLAB.
- To study the dynamic behavior of the model based on the results obtained.
- To study and discuss the comparison between two assumption constant molar flow and non constant molar flow.

1.4 The Relevancy of Project

Among the advantages of this project are one can study the dynamic responses and behavior of CDU based on the more accurate model. Also, student will be able to see the details of the calculation and complexity behind the multicomponent distillation simulation such as HYSYS which is widely use in the university and industry. Lastly, student will be able to study and familiarize with modern computer programming language, MATLAB which is now considered as a standard tool at most universities and industries worldwide.

1.5 Scope of Work

Firstly, preview on other research papers, journals and book is done in other to understand the scope of this research and also the theory behind crude distillation unit. Secondly, to start developing model, some assumptions regarding the model must be clearly specified. Then, Rigorous dynamic model for each types of stage is developed considering mass balance, energy balance equilibrium and flow dynamic (linearized Francis Weir Formula). Rigorous models based on the two assumptions, constant and non constant molar flow are developed and studied. For constant molar flow, only covers mass and component balance whereas, for non constant molar flow it is necessary to cover energy balance. After develop Rigorous, in other to get the input and properties for CDU model HYSYS 3.2 is used and from the HYSYS, boiling point data and feed inlet fraction can be determined. Then, MATLAB is used to solve the constant molar flow model to study the dynamic characteristic of the model. The dynamic studies involving changes in feed flow rate and feed composition are carried out and from those results the dynamic behavior of the system is obtained. The flow of research work can be summarized as Figure 1.1 below:-

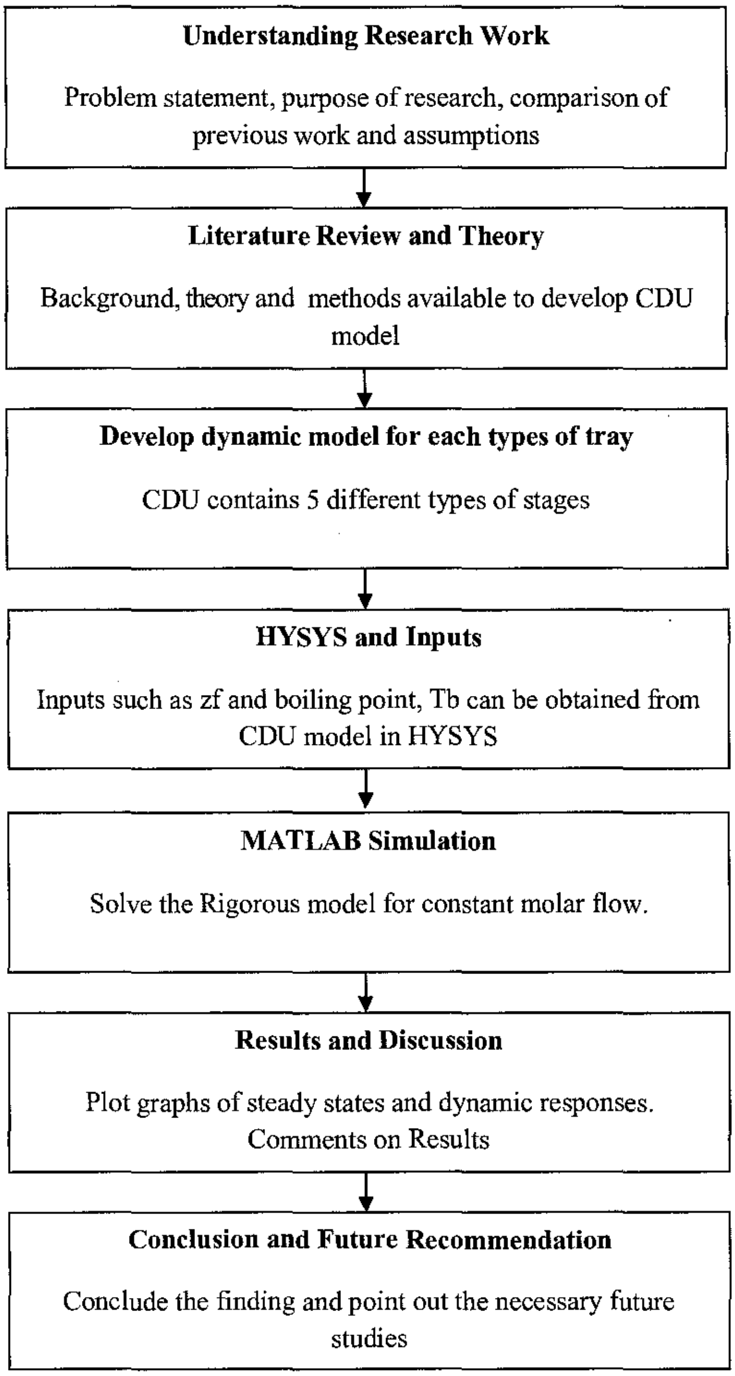

Figure 1.1: Work Flow of Project

CHAPTER 2

LITERATURE REVIEW

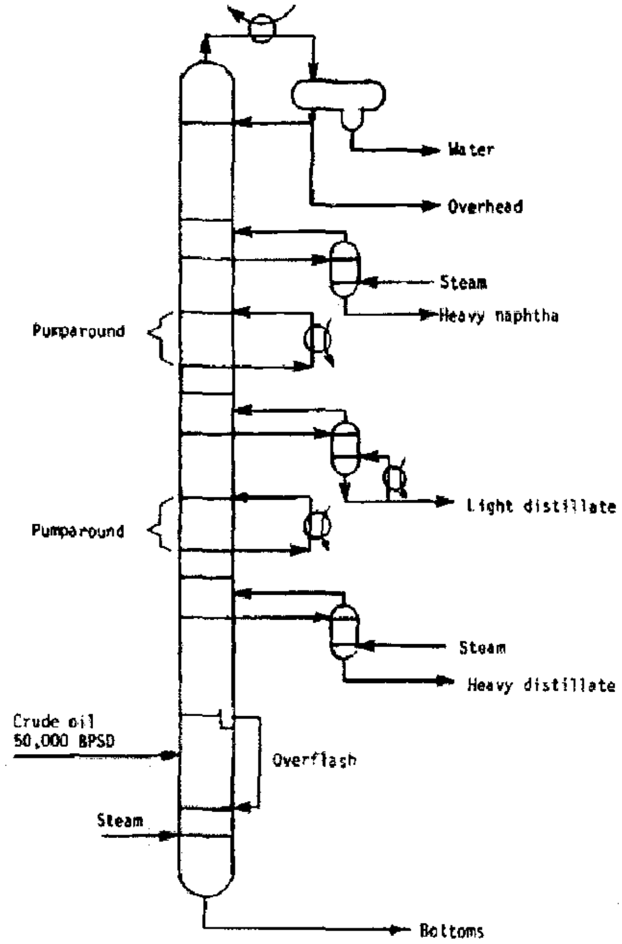

Figure 2.1: Crude Distillation Column (CDU)[8]

2.1 Background of CDU

In the refineries, the crude oil feedstock is a very complex multi-component mixture that must be separated and yields of pure chemical compounds are not expected, only groups of compounds within a relatively small range of boiling points, which are called *fractions*.

The aim of a CDU is to separate the complex mixture of hydrocarbon components into many products of different compositions. The physical principle of separation in distillation is the difference in the volatility of the components. The crude oil fractionators does not produce products having a single boiling point; rather, it produces fractions having boiling ranges. For examples, the naphtha cut, as that fraction is called, contains many different hydrocarbon compounds. Therefore it has an initial boiling point of about 35 °C and a final boiling point of about 200 °C. Each cut produced in the fractionating columns has a different boiling range. At some distance below the overhead, the next cut is withdrawn from the side of the column and it is usually the jet fuel cut, also known as a kerosene cut. The boiling range of that cut is from an initial boiling point of about 150 °C to a final boiling point of about 270 °C, and it also contains many different hydrocarbons. The next cut further down the tower is the diesel oil cut with a boiling range from about 180 °C to about 315 °C. The boiling ranges between any cut and the next cut overlap because the distillation separations are not perfectly sharp. After these come the heavy fuel oil cuts and finally the bottoms product, with very wide boiling ranges. All these cuts are processed further in subsequent refining processes.

2.2 Rigorous Model

Models are often classified as “rigorous” or “simplified” models. Rigorous models for equilibrium stages consist of mass and energy balance which include some kind of flow and pressure dynamic as well as the thermodynamic relations. The flow dynamic describe the changes in liquid holdup on a stage because of variations in liquid and vapor flow, while the pressure dynamic primary influence the vapor holdup on a stage. Considering the stage design (see Figure 2.2) of a column the liquid holdup has (sometimes) to be split into liquid on the tray and downcomer which result in twice as much state per stage. Nevertheless, even in the most rigorous model certain simplifications as thermal and mechanical equilibrium or assumption of perfect mixing in the phases are introduced. The thermodynamic equilibrium (vapor liquid equilibrium) can be corrected by introducing a simple Murphree tray efficiency for each component. Commonly, the effect of heat losses to the surroundings and the dynamic of the column structure are neglected. [11]

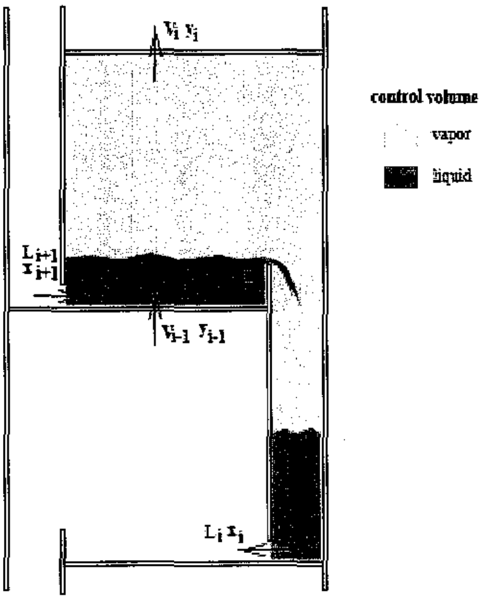

Figure 2.2: Control volume on a stage

Assumptions for an equilibrium based on the stage model:

- Perfect mixing in both liquid and vapor phase
- Thermodynamic and mechanical equilibrium (assume 100 % tray efficiency)
- Neglect heat loss and thermal capacity of column structure
- Consider only normal operation (*e.g.* no flooding, weeping)

2.3 Constant molar flow and non-constant molar flow models

Constant molar flow is defined as the molar vapor and liquid flows from each stage is constant. This can only be true where the component molar latent heat of vaporization are the same and the together with the specific heat are the same over the range of temperature of the column, there is no significant heat of mixing and heat loss is negligible, whereas non constant molar flow is the molar vapor and liquid flow is not constant. Therefore, energy balance need to be solved and cannot be neglected

Derivation of constant molar flow model

This derivation is included because no rigorous derivation of this common assumption is included in the recent literature. Assumptions (S.Skogestad, 1997):

1. References state of energy is pure components as saturated liquids at a given references pressure.
2. The column pressure is constant and equal to the references pressure
3. Negligible heat of mixing such that $h_{Lj} = \sum_i x_{ij} \, c_{PLi}(T_j - T_{bpi})$ where T_{bpi} is the boiling point of pure component i at reference pressure.
4. All components have the same value of liquid molar heat capacity c_{PLi}
5. The tray temperature, T_j, is the average of components boiling point. $T_j = \sum_i x_j \, T_{bpi}$. This assumptions gives $h_{Lj} = 0$ and thus $dh_{Lj}/dt = 0$ on all stages.The constant molar flow case is derived by assuming in addition that

6. The vapor phase is ideal and all components have the same heat of vaporization. $h_i^{vap} = h^{vap}$, where h_i^{vap} is the heat of vaporization of pure component i at the column pressure. Then, $h_{Vi} = h_i^{vap} + \sum_i x_{ij}\, c_{PVi}(T_j - T_{bpi})$
7. c_{PVi} is equal for all components such that the last term is zero (as for the liquid). Then we have on all stages, $h_{Vj} = h^{vap}$ and the energy balance becomes; $V_j = V_{j-1}$

2.4 Francis's weir formula and Simplication of Liquid Flow

Dynamics Francis Weir Formula

The Francis weir formula is well known to represent the liquid flow dynamic in each tray.

$$L_j = f(M_j)$$

$$L_j = 3.33\, l_w (h_{ow})^{1.5} \tag{1}$$

$$h_{ow} = \frac{M_j m_j}{\rho_j A} - h_{weir} \tag{2}$$

Where;

m_j=molecular weight at jth stage liquid.

ρ_j=density of jth stage liquid

h_{weir} = height of weir

A= Area of a tray

Simplification of Liquid flow dynamic

Details on the liquid flow dynamics for trayed distillation columns are published by Rademaker *et al.* (1975). Linearized tray hydraulics or linearized Francis Weir is presented by Rademaker *et al.* (1975) and Skogestad (1988).

Liquid flows are given by Franci's Weir Formula L (j) =K*Mow (j) $^{1.5}$ where the liquid flow, L (j), dependent only on the holdup over the weir Mow (j). M (j) = Mow (j) + Muw (j) (Total holdup = holdup over weir + holdup below weir)

Liquid flows below feed (Kmol/min),
For j=2.... NF;

$$L_j = K_{bf}(M_j - M_{UW})^{1.5} \tag{3}$$

$$K_{bf} = \frac{Lo + F}{(M_0 - M_{UW})^{1.5}} \tag{4}$$

Liquid flows above feed (Kmol/min),
For j=NF+1...NT-1;

$$L_j = K_{af}(\mathrm{M_j} - \mathrm{M_{UW}})^{1.5} \tag{5}$$

$$K_{af} = \frac{Lo}{(M_0 - M_{UW})^{1.5}} \tag{6}$$

Where;

K_{bf} Constant below feed
K_{af} Constant above feed
M_{UW} Holdup under weir (kmol)
L_j Liquid flows (kmol/min)

2.5 Vapor-Liquid Equilibrium Relation

Since petroleum fractions are complex mixtures of hydrocarbons, single pure component thermodynamics is not applicable. In estimation of these thermodynamic properties, the use of empirical or semi-empirical correlations is quite popular. Some of the commonly used techniques are based on the cubic equation. Thermodynamic properties of vapor–liquid mixtures are generally predicted by calculating deviations from ideality of both the vapor and liquid phases by using any of the above mentioned equations of state. The equation of state is applied only to the vapor phase while liquid phase deviations from ideal solution behavior are calculated using thermodynamic excess functions. For a rigorous crude distillation, it is important to use prediction models for the thermodynamic properties, which are continuous functions, and are applicable in the entire range of temperature (0–500) °C for the lighter as well as the heavier components. Additionally, to ensure smooth convergence, there should not be any discontinuity of real roots for the equations of state in the entire domain of operation of the crude distillation unit[4]. Therefore, in this report, equilibrium constant K is calculated by equation (4) below.

The vapor phase composition in equilibrium with liquid phase is given by;

$$y_{i,j} = K_{i,j} x_{i,j} \tag{7}$$

$$\sum_{i=1}^{C} y_{i,j} = 1 \quad j = 1, 2 \ldots. N \tag{8}$$

$$\sum_{i=1}^{C} x_{i,j} = 1 \quad j = 1, 2 \ldots. N \tag{9}$$

$$K_{i,j} = K_{i,j}[T_j, P_j, x_j, y_j]$$

Equilibrium constant K equation [4] can be written as;

$$K_i = \frac{p_i^{\circ}}{P} = \frac{p_i^{c}}{P} \exp[(1 + w_i) f(T_{r,i})] \tag{10}$$

The relation of the equation and equation of state approach is based on figure below;

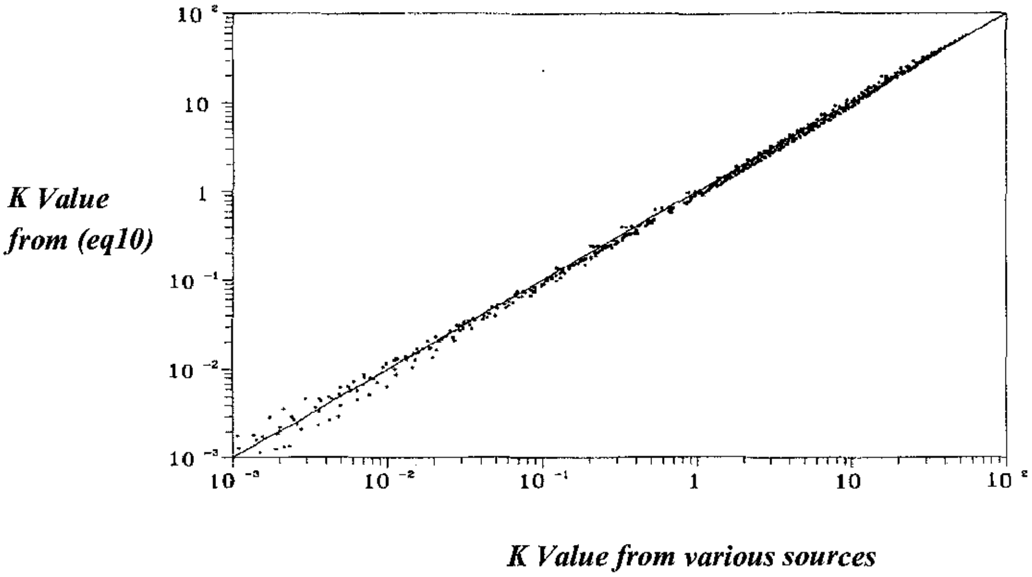

Figure 2.3: Parity plot for calculated values of equilibrium constants with data obtained from various sources. [4]

The various sources to calculate K is based on Peng Robinson, Lee Kesler and BrownK_{10} methods.

CHAPTER 3: METHODOLOGY

The first step of modeling CDU is by developing the MESH equations for each type of stage model which representing the whole column. Referring to figure 3.1 below, there are five types of stages will be considered which are simple j^{th} stage, feed stage, total condenser stage, reboiler stage and intermediate stage (side product).

3.1 Overall Column model

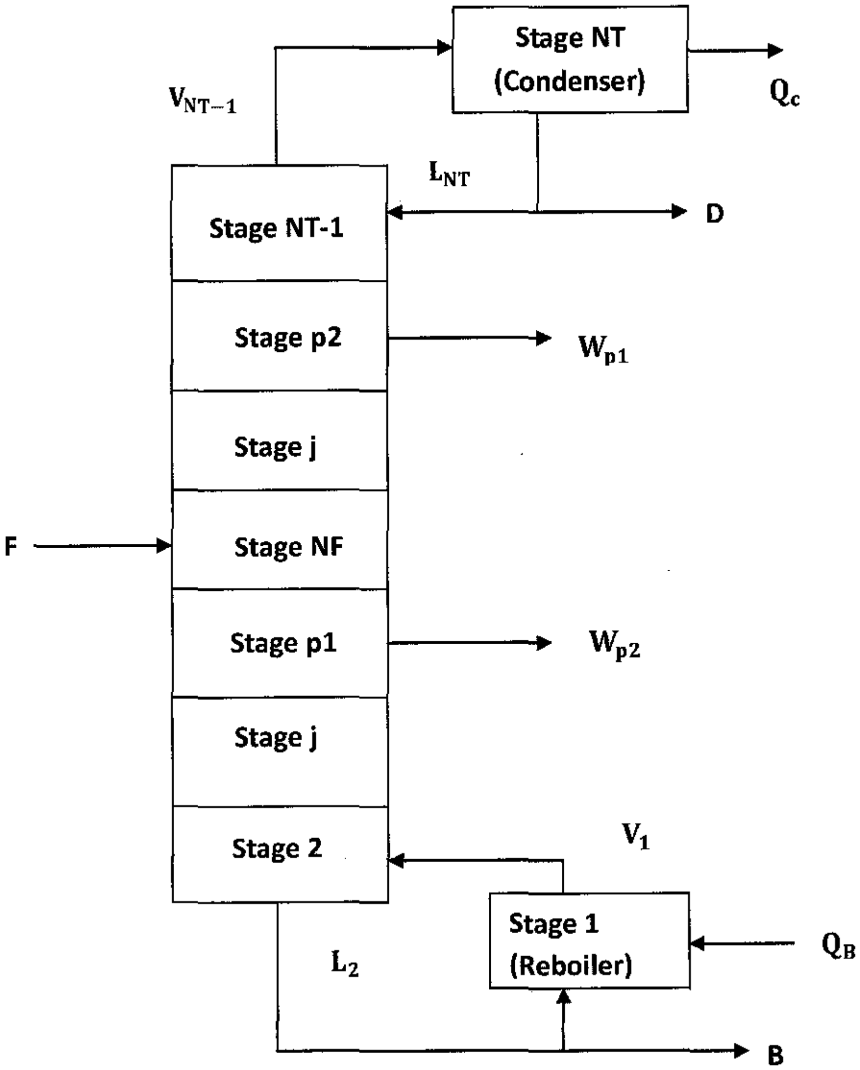

Figure 3.1: Overall CDU column model

3.2 The Model and Balance Equations

Assumptions

1. The liquid on the tray is incompressible.
2. Tray vapor holdups are negligible. Entrainment flow will not considered
3. Vapor and liquid are in equilibrium.
4. Liquid flow dynamic is modeled by Francis Weir Formula
5. NC components (multicomponent mixtures), component NC is the heavy component.
6. NT is condenser stage
7. Total Condenser.

The balance equations for simple jth stage

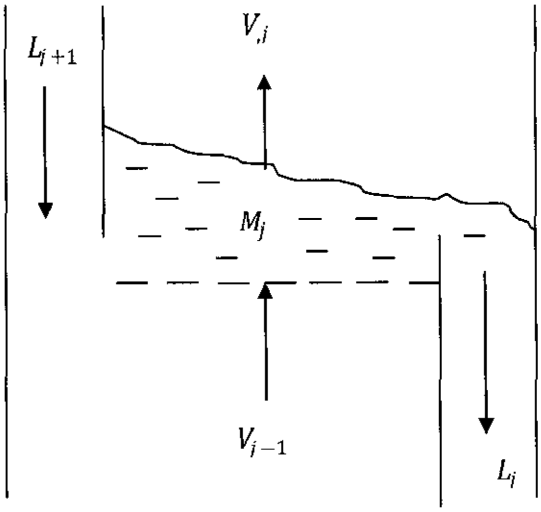

Figure 3.2: Schematic Diagram for Simple *jth* Stage Model

$$\frac{dM_j}{dt} = L_{j+1} + V_{j-1} - L_j - V_j \tag{11}$$

$$\frac{dM_j x_{j,i}}{dt} = L_{j+1}x_{j+1,i} + V_{j-1}y_{j-1,i} - L_j x_{j,i} - V_j y_{j,i} \quad i = 1,2...NC \tag{12}$$

$$\frac{dh_j}{dt} = L_{j+1}h_{j+1} + V_{j-1}H_{j-1} - L_j h_j - V_j H_j \tag{13}$$

$$\frac{M_j dT}{dt} = L_{j+1}\left(T_{j+1} - T_j\right) + V_{j-1}\left(T_{j-1} - T_j + H_j/C_{p,j}\right) - V_j\left(\frac{H_j}{C_{p,j}}\right) \tag{14}$$

The balance equations for feed stage (j=NF)

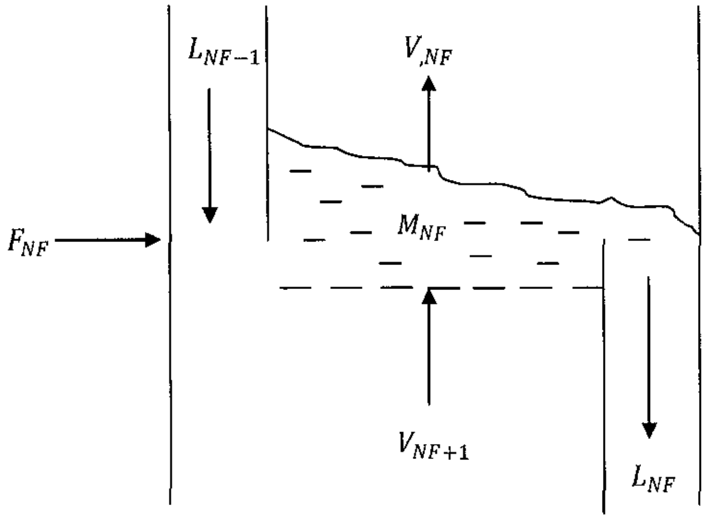

Figure 3.3: Schematic Diagram for Simple feed (j=NF) Stage Model

$$\frac{dM_{NF}}{dt} = F_{NF} + L_{NF-1} + V_{NF+1} - L_{NF} - V_{NF} \tag{15}$$

$$\frac{dM_{NF}x_{NF,i}}{dt} = F_{NF}z_{NF,i} + L_{NF-1}x_{,NF-1,i} + V_{NF+1}y_{NF+1,i} - L_{NF}x_{NF,i} - V_{NF}y_{NF,i}$$

$$i = 1,2 \ldots NC \tag{16}$$

$$\frac{dM_{NF}h_{NF}}{dt} = F_{NF}h_{NF} + L_{NF-1}h_{,NF-1} + V_{NF+1}H_{NF+1} - L_{NF}h_{NF} - V_{NF}H_{NF} \tag{17}$$

$$\frac{dM_{NF}T_{NF}}{dt} = \frac{dM_{NF}}{dt} + F_{NF}\left(T_{feed} - T_{NF}\right) + \frac{F(1-q_{NF})H_{NF}}{C_{p,NF}} \tag{18}$$

The balance equations for total condenser (j=NT)

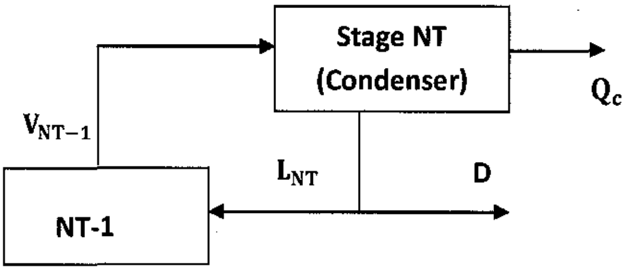

Figure 3.4: Total Condenser (j=NT) Stage Model

$$\frac{dM_{NT}}{dt} = V_{NT-1} - (L_{NT} + D) \tag{19}$$

$$\frac{dM_{NT}x_{NT,i}}{dt} = V_{NT}y_{2NT,i} - (L_{NT} + D)x_{D,i} \quad i = 1,2\ldots NC \tag{20}$$

$$\frac{dM_{NT}h_{NT}}{dt} = V_{NT-1}H_{NT-1,i} - (L_{NT} + D)h_{NT} - Q_c \tag{21}$$

$$\frac{M_{NT}dT_{NT}}{dt} = V_{NT-1}(T_{NT-1} - T_{NT}) + \frac{H_{NT}}{C_{p,NT}(V_{NT-1} - D\,)} \tag{22}$$

The balance equations for reboiler (j=1)

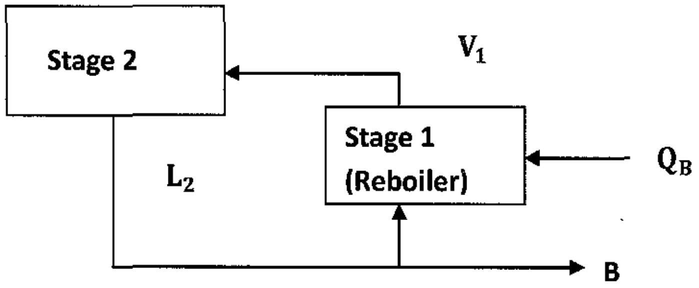

Figure 3.5: Reboiler (j=1) Stage Model

$$\frac{dM_1}{dt} = L_2 - (V_1 + B) \tag{23}$$

$$\frac{dM_1 x_{1,i}}{dt} = L_2 x_{2,i} - V y_{1,i} - B x_{2,i} \quad i = 1,2 \ldots NC \tag{24}$$

$$\frac{dM_N h_N}{dt} = L_2 h_2 - V_1 H_1 - B h_2 + Q_B \tag{25}$$

$$\frac{M_1 dT_1}{dt} = L_2 (T_2 - T_1) + \frac{H_1}{C_{p,1}(B - V_1)} \tag{26}$$

The Balance equations for side product (j=p)

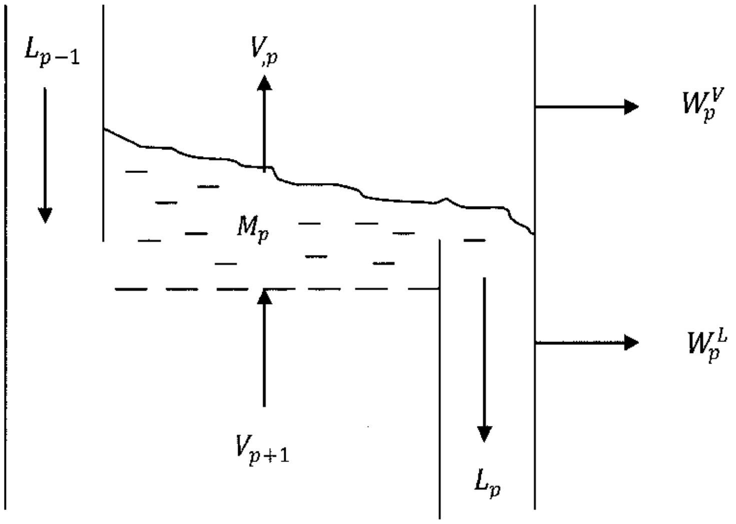

Figure 3.6: Schematic Diagram for Side Product (j=p) Stage Model

$$\frac{dM_p}{dt} = L_{p-1} + V_{p+1} - \left(L_p + W_p^L\right) - \left(V_p + W_p^v\right) \tag{27}$$

$$\frac{dM_p x_{p,i}}{dt} = L_{p-1}x_{j-1,i} + V_{p+1}y_{p+1,i} - \left(L_p + W_p^L\right)x_{p,i} - \left(V_p + W_p^v\right)y_{p,i} \tag{28}$$

$i = 1,2 \dots NC$

$$\frac{dM_p h_p}{dt} = L_{p-1}h_{p-1} + V_{p+1}H_{p+1} - \left(L_p + W_p^L\right)h_p - \left(V_p + W_p^v\right)H_p \tag{29}$$

Linearized Liquid Flow Dynamic

The linearizd liquid from equation (eq.3, 4, 5, and 6) will be applied

Liquid flows below feed, for j=2.... NF;

$$L_j = K_{bf}(M_j - M_{UW})^{1.5}$$

$$K_{bf} = \frac{Lo + F}{(M_0 - M_{UW})^{1.5}}$$

Liquid flows above feed, for j=NF+1...NT-1;

$$L_j = K_{af}(\mathrm{M_j} - \mathrm{M_{UW}})^{1.5}$$

$$K_{af} = \frac{Lo}{(M_0 - M_{UW})^{1.5}}$$

Simplified Vapor Flow

Based on the derivation of section 2.3, the vapor flow can written as

Vapor flows below feed (Kmol/min), for j=1.... NT-1;

$$V_j = V_{j-1} \tag{30}$$

Vapor flows below feed (Kmol/min), for j=NF.... NT-1;

$$V_j = V_{j-1} + (1 - q_F)F \tag{31}$$

Equilibrium & Summation Equations

The equilibrium equation, equation (8-10) in section 2.5 is applied:

$$y_{i,j} = K_{i,j} x_{i,j}$$

$$K_i = \frac{p_i^{\circ}}{P} = \frac{p_i^c}{P} \exp[(1 + w_i) f(T_{r,i})]$$

3.3 HYSYS and Inputs

CDU Model Data and Properties for MATLAB Inputs

In this research, CDU products are assumed to be the typical ones which are Gas, Naphtha, Kerosene, Diesel, AGO and Residue. In order to get the properties of these products, firstly crude distillation unit has been developed in HYSYS environment.

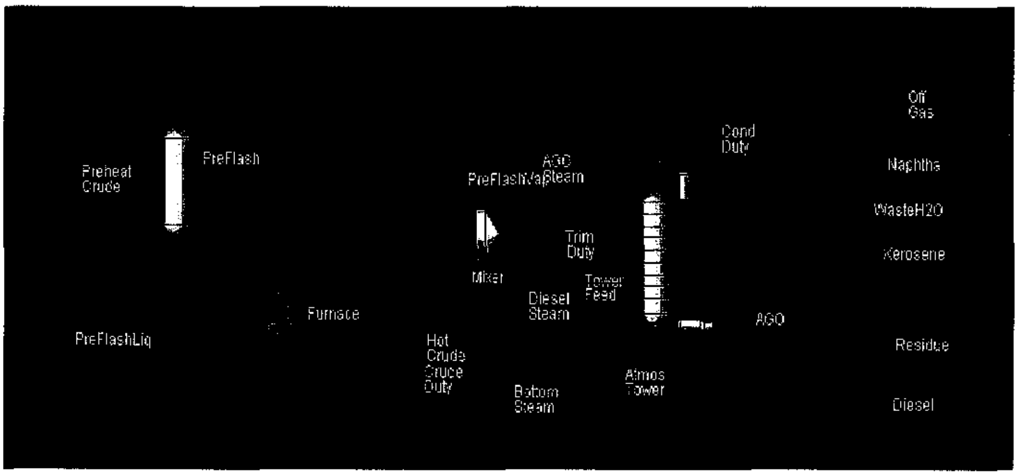

Figure 3.7: Crude Distillation Unit in HYSYS

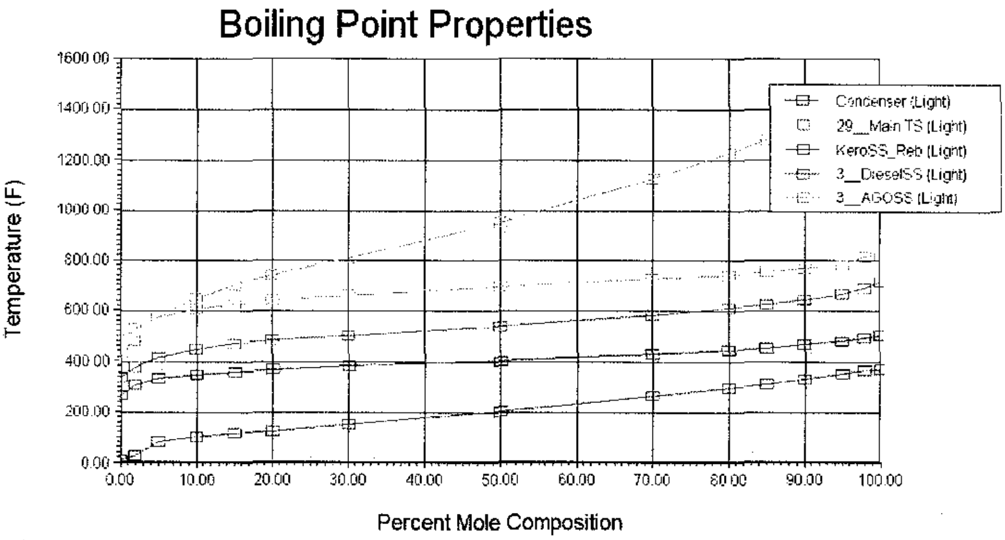

Figure 3.8: Boiling Point Properties extracted from HYSYS

Name	**Feed**	**Off Gas**	**Naphtha**	**Kerosene**	**Diesel**	**AGO**	**Residue**
Vapor Fraction	0.2937	1	0	0	0	0	0
T (F)	450	107.3	107.3	4575	486.8	571.6	669.1
Pressure (psia)	75	19.7	19.7	29.84	30.99	31.37	32.7
Molar Flow (lb/hr)	6214	4.473×10^{-5}	2822	701.9	1114	200.4	1397
Mass Flow (lb/hr)	1.282×10^{8}	2.3×10^{-3}	2.474×10^{5}	1.115×10^{5}	2.429×10^{5}	5.945×10^{4}	6.216×10^{5}
LVF (bbl/day)	1×10^{5}	2.612×10^{-4}	2.3×10^{4}	930	1.325×10^{4}	4500	4.398×10^{4}
Heat Flow (Btu/hr)	-1.912×10^{8}	-2.296	-2.331×10^{8}	-8.09×10^{7}	-1.772×10^{8}	-3.882×10^{7}	-3.647×10^{8}

Table 1: Material Stream and Properties of CDU Products based on HYSYS Aspen

Determination of Feed fraction, z_f

Name of Fraction	Mole Fraction , z_f
Off gas	0.01
Naphtha	0.45
Kerosene	0.113
Diesel	0.18
AGO	0.05
Residue	0.22

Table2: Fraction of Product Cuts in Feed (Crude)

As shown in Table 2, mole fraction for feed, z_f can be obtained from Table 1. These data will be used as input data in MATLAB computation.

Determination of Equilibrium Constant, *K*

Name of Fraction	T_{bp} (F)/(°C)/(°K)	Equilibrium Constant
Off gas	60/15/288	1.9
Naphtha	158/70/343	3.9
Kerosene	360/182/455	1
Diesel	554/290/563	5
AGO	644/340/613	8
Residue	980/527/800	0.49

Table3: Equilibrium Constant *K* for each Pseudo-component (Crude)

Based on Table 3, the boiling point temperature for each cut is important to determine the equilibrium constant, K. The value of K can be obtained by figures below. These figures of equilibrium constant, K vs T_{bp} is based on the modified equation of equilibrium constant as mentioned in section 2.4, equation (10)

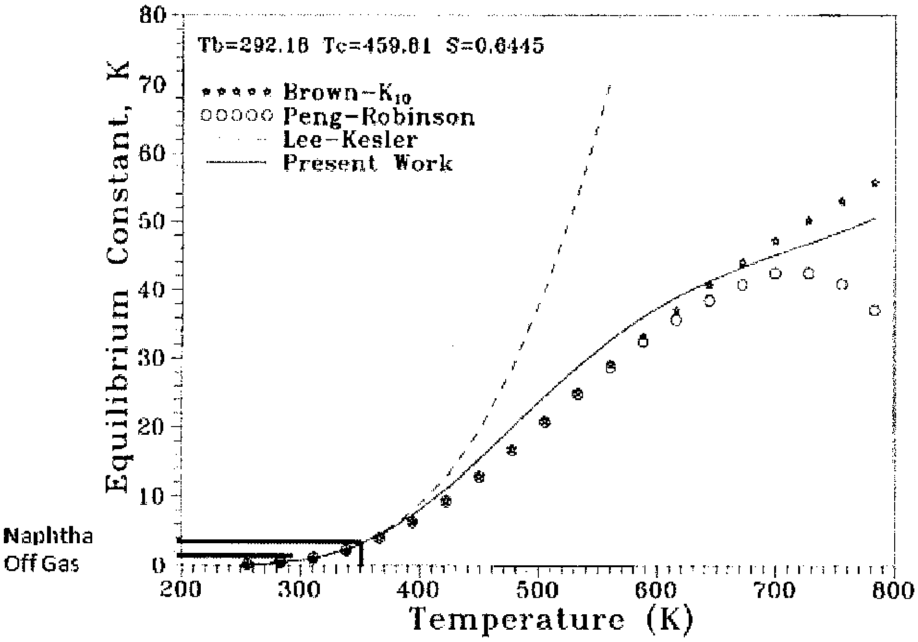

Fig. 2. Comparison of equilibrium constants calculated by various methods for a low boiling pseudo-component (T_b = 292.18 K).

Figure 3.9: Equilibrium Constant versus T_b for a low boiling pseudo-component (Tb=292K) [4]

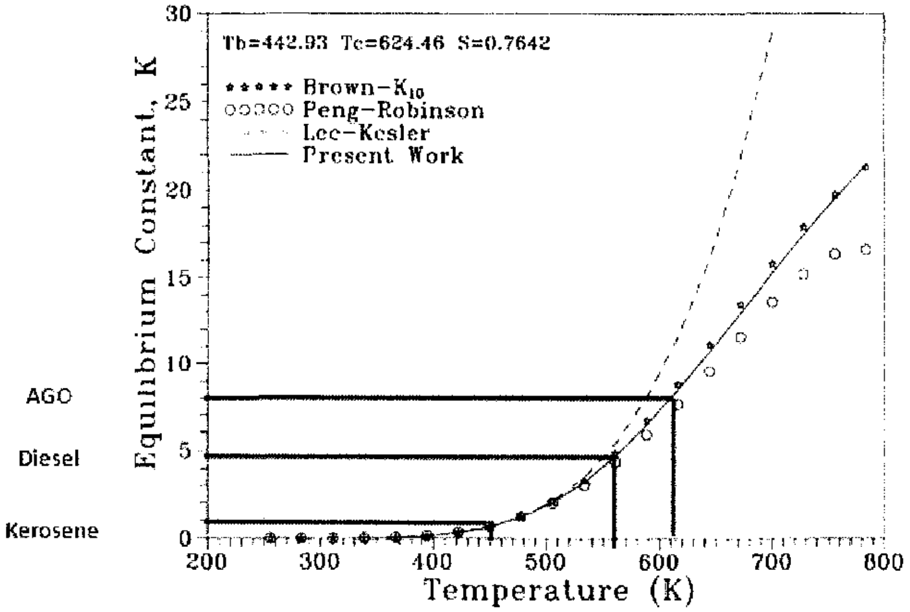

Fig. 3. Comparison of equilibrium constants calculated by various methods for a middle range boiling pseudo-component (T_b = 442.93 K).

Figure 3.10: Equilibrium constant versus Tb for middle range boiling pseudo-component (Tb=443K) [4]

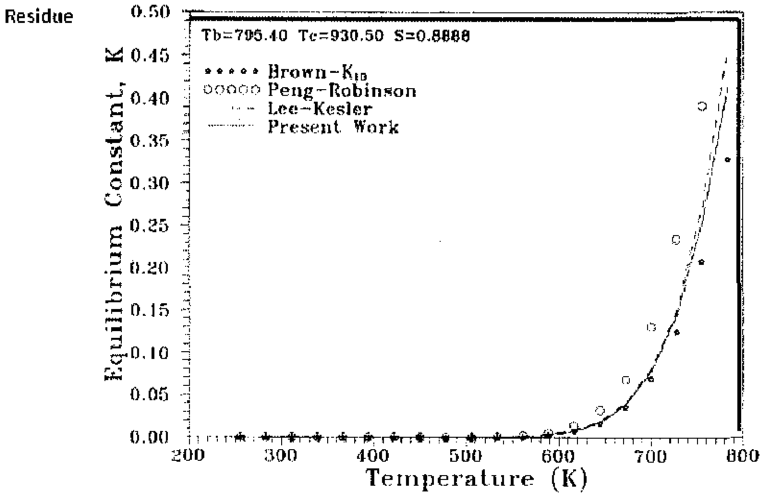

Fig. 4. Comparison of equilibrium constants calculated by various methods for a high boiling pseudo-component (T_b = 795.40 K).

Figure 3.11: Equilibrium constant versus Tb for high boiling pseudo-component (Tb=795K) [4]

3.4 MATLAB Computational Method implemented in the present model (Constant Molar Flow Model)

Refer Appendix A for detail of MATLAB coding. In other to simplify the coding, several steps of computational MATLAB is summarized as below;

Step 1: Define Function,xprime

- xprime is vector with time derivatives of all states

  'xprime= crudeA (t, X, U)'
- Where t is time ,X is state for composition and hold up and U is disturbance vector

Step 2: Input Initial Data

- **Simulation data**: *simulation time, t and state, X.*

- **Operating data**: *reflux L; boil up V, top or distillate product D, bottom product B, side product W (liquid and vapor), K (equilibrium constants for the mixtures)*

- **Disturbance:** *Feed rate F, feed composition z*

- **Column specification data**: *Total number of trays NT, Feed tray NF, Side product tray NP. (These data can be changed for different column)*

Step2: Evaluate the model

- **Equilibrium relation**: *K value*

  $y_{i,j} = K_{i,j} x_{i,j}$

- **Vapor flows**: *Simplified Energy balance*

- Vapor flows below feed (Kmol/min), for j=1.... NT-1;

  $V_j = V_{j-1}$

- Vapor flows below feed (Kmol/min), for j=NF.... NT-1;

  $V_j = V_{j-1} + (1 - q_F)F$

- **Liquid flow**: *linearized liquid flow dynamic formula*

- Liquid flows below feed, for j=2.... NF;

$$L_j = K_{bf}(M_j - M_{UW})^{1.5}$$

$$K_{bf} = \frac{Lo + F}{(M_0 - M_{UW})^{1.5}} = 29.65032$$

- Liquid flows above feed , for j=NF+1...NT-1;

$$L_j = K_{af}(\mathrm{M_j} - \mathrm{M_{UW}})^{1.5}$$

$$K_{af} = \frac{Lo}{(M_0 - M_{UW})^{1.5}} = 21.65032$$

- **Evaluate time derivatives from material balance for jth stage**: *liquid hold up and component hold up.*
  - Correction factor: *feed stage, total condenser stage, reboiler stage and side product stage.*

- **Compute the derivatives for material and composition.**
  - By applying chain rule,

$$\frac{d(Mx)}{dt} = x\frac{dM}{dt} + M\frac{dx}{dt}$$

$$\frac{dx}{dt} = (\frac{d(Mx)}{dt} - x\frac{dM}{dt})/M$$

Step 3: Run the simulation to get initial steady state data from which to do the nonlinear simulations and save file as 'crudeA_ss'.

- The data includes the initial steady-state molar compositions of components 1 to NC-1 at all NC stages and molar liquid holdups at all NC stages.

Step 4: Dynamic response to increase the feed rate

- Change the feed rate (+1%) from 10.00 Kmol/min to 10.1 Kmol/min and then save file as 'crude_F1'.
- Repeat for change in federate +10%

Step 5: Plot Graph

- After saving the file, we can simulate using ordinary differential equation (ode15s) and put time interval. Referring to the appendix, the graphs plotted include;
- Figure 1: Distillate composition (light) versus time (xD vs t)
- Figure 2: Reboiler composition (light) versus time (xB vs t)
- Figure 3: Reboiler Holdup versus time (MB vs t)
- Figure 4: composition profile through plate number (xprofile0 vs plate number)
- Figure 5: composition versus time

All the steps can be repeated for increase in feedrate 10 %, change in feed fraction and etc.

CHAPTER 4

RESULTS AND DISCUSSIONS

Consider a crude mixture to be fed to a crude distillation column containing 38 theoretical stages, NT including reboiler (stage 1) plus a total condenser. The assumptions made are the pressure is constant on all trays (constant molar flow). the vapor and liquid leaving each tray are in equilibrium (i.e., tray efficiency is 100%), no vapor holdup, liquid flow dynamic modeled by Francis Weir formula, total condenser and the feed is assumed to be mixed into feed stage. The CDU feed, assumed to be saturated liquid and the total components, NC is 6 which are 1% Off gas, 45% Naphtha, 11.3% Kerosene, and 18% Diesel, 3.3% AGO and 22% Residue. Feed flow rate is set equal to 10 kmol/min. The feed is entered at the 15 th stage. Disturbances are feedrate, feed composition and feed liquid fraction. In this part, most of the results will discuss about light components (Off Gas, light Naphtha and water) at distillate and reboiler stage. These components are distillate since the condenser is assumed to be total reflux.

4.1 Steady States Results

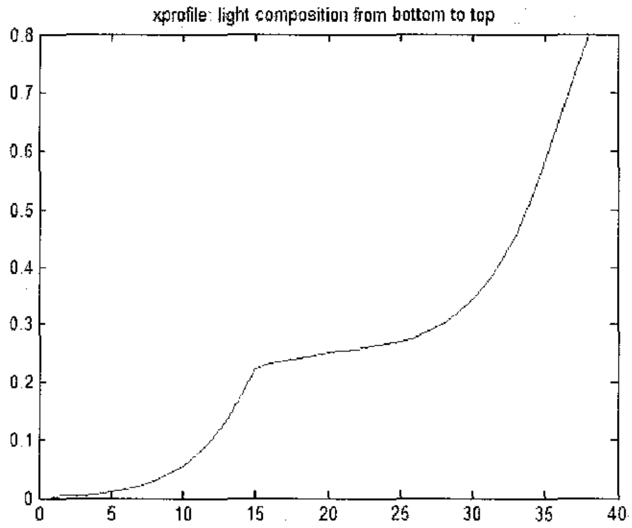

Figure 4.1 (a): Composition profile from bottom to top

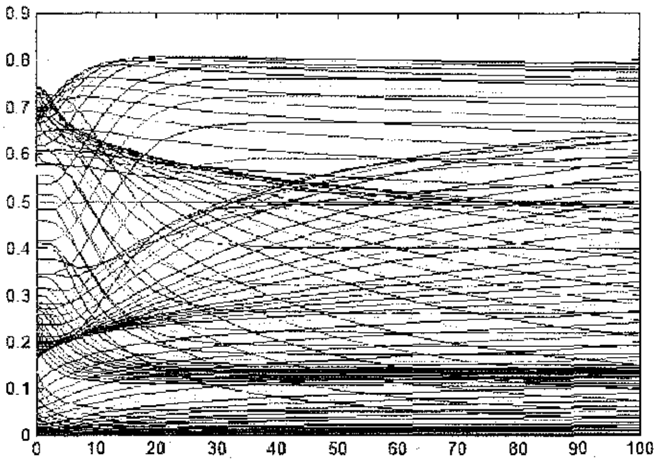

Figure 4.1 (b): Composition profile versus time

From the graph 4.1 (a), figure shows the composition profile from bottom to top. This profile shows the nonlinearity especially at the bottom of the column when N < NF (15th Stage). The graph starts to be linear at the top of the column NT, (stage 38). The nonlinearity happens because the effect of changes depends strongly on the magnitude of the change and on the operating point. The primary reason for this is the nonlinear VLE. However, Skogestad [10] mentioned in his book that both at steady state and especially dynamically, is much less depending on operating point if we instead consider logarithm composition defined as the logarithm between the ratio of the key components. The composition profile also shows non-optimal feed location. The optimal feed location can be found by using Fenske Formula.

4.2 Dynamic Responses-Change in Feed Rate

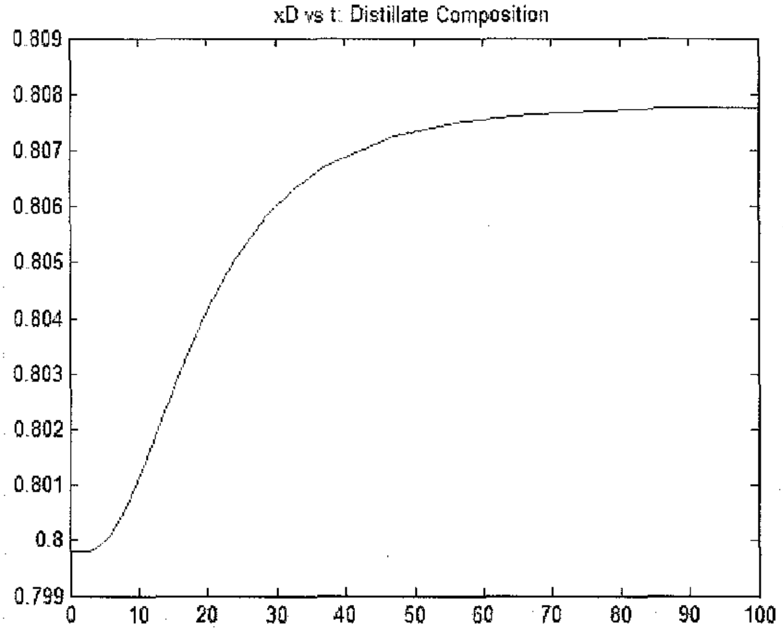

Figure 4.2(a): Simulated responses in distillate composition versus time for +1% step change in F (xD vs t)

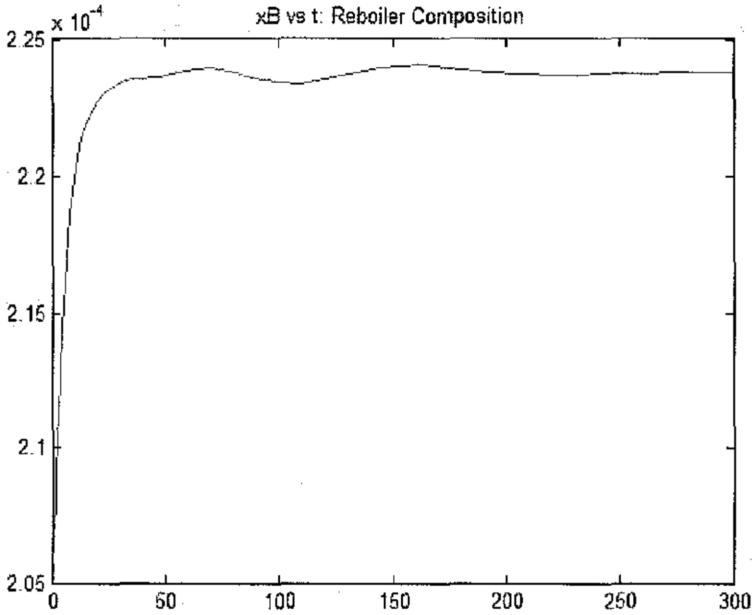

Figure 4.2 (b): Simulated Responses in Reboiler Composition versus time for +1% step change in F (xB vs t)

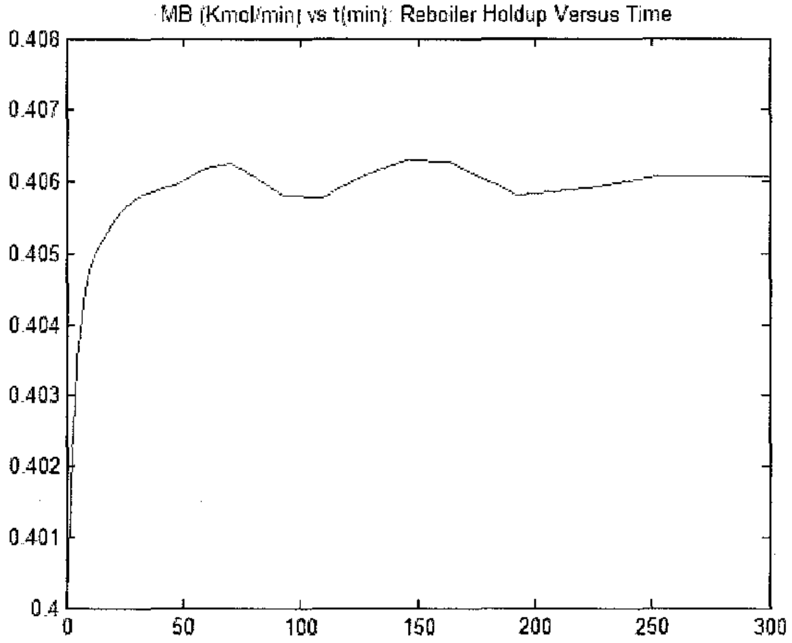

Figure: 4.2(c): Simulated Responses in Reboiler Holdup versus time for +1% step change in F (MB vs. t)

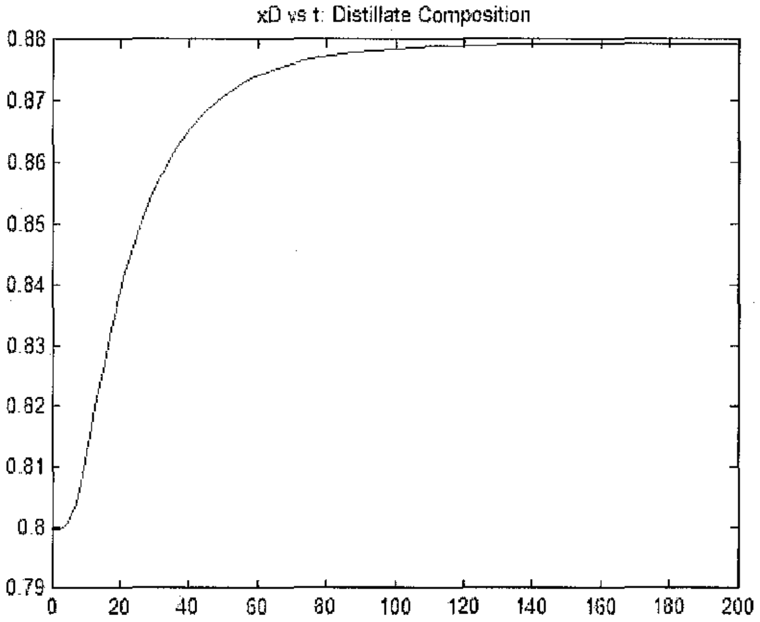

Figure 4.2(d): Simulated responses in distillate composition versus time for +10% step change in F (xD vs. t)

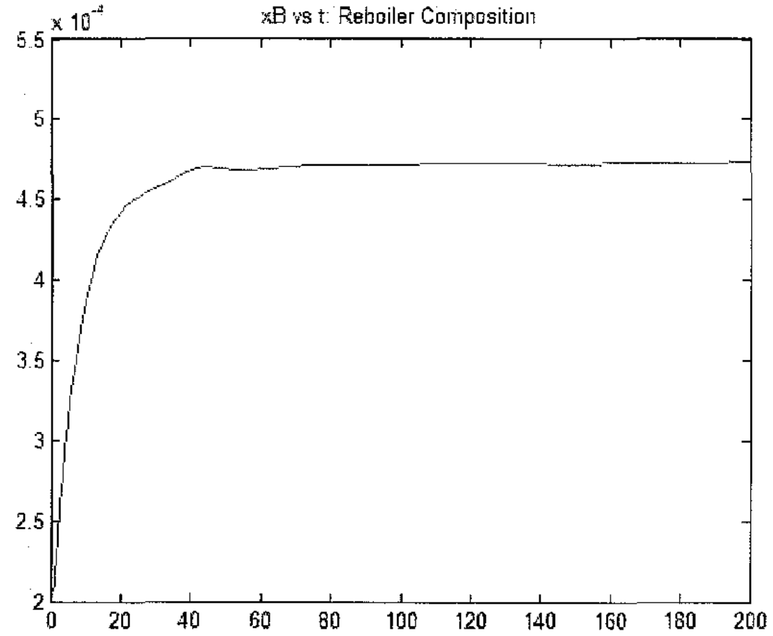

Figure 4.2 (e): Simulated Responses in Reboiler Composition versus time for +10% step change in F (xB vs. t)

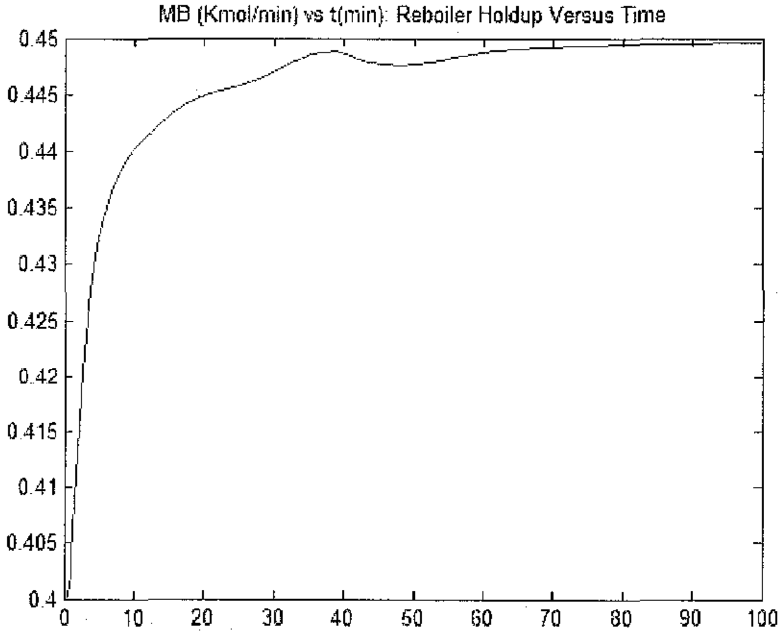

Figure 4.2(f): Simulated Responses in Reboiler Holdup versus time for +10% step change in F (MB vs. t)

Figure 4.2 (a-c) shows the responses of distillate composition, bottom composition and reboiler holdup with increase in feedrate 1%. As a result, the distillate composition, xD is increased by 1% (from 0.8 to 0.808), the bottom composition, xB is increased by 9.7% from (2.05 x 10^{-4} to 2.25 x10^{-4}) and reboiler holdup, MB increases by 1.5 %(from 0.4 to 0.406).

For 10% increased in federate from figure 4.2(d-f), xD is increased by 10% (from0.8to0.88), xB is increased by 150% (from 2.05x10'4 to5.5x10^{-4}) and MB is increased by 15% (from 0.4 to 0.45). The time constant (at 63.2% change before reaching new steady state) calculated for xD,xB and MB are 25 minutes, 15 minutes and 10 minutes).

From this result, xD responses linear to the change in feedrate responses. Increases in feedrate give large upset to the xB and MB. This is because increased in feedrate goes down to the bottom of the column and increased the bottom flows.

From the time constant, τ, calculated from the figures above, MB shows fast responses towards change in feedrate compare to composition. This is because feedrate is the external flow. Based on Skogestad [10], change in external flow such as F, D and B usually have large effecr on the compositions and holdup, xD, xB and MB.

In overall view, the feed flow rate is the disturbances affecting the product compositions in a distillation column. The changes in these disturbances shift the composition profile through the column resulting in a large upset in the product compositions. All the figures show the stability and reasonable accuracy of steady states.

CHAPTER 5

CONCLUSSION AND FUTURE RECOMMENDATION

5.1 Conclusions

Modeling of CDU is today the foundation to almost any operation including design, control, planning and retrofitting of the refinery plant. This research shows Rigorous model of constant molar flow of CDU is successfully developed and solved in MATLAB environment. Liquid flow dynamic modeled by Franci's Weir formula is able to be applied to model the liquid flow dynamic and also improves the accuracy of the model. Based on the model developed, one can see the complexity of the CDU model. Besides that, one also can study the dynamic behavior of CDU model. Based on the dynamic studies, it can be concluded;

- Steady states and dynamic simulation results indicated the nonlinearity of the process.
- Current model had provided steady states with a reasonable accuracy.
- Increases in feed flowrate results in large upset in composition.
- Linearized Francis Weir formula has improved the accuracy of the model.
- Reboiler holdup rensponses is faster than composition responses
- xD responses is linearly depend on feedrate response change.
- xB is effected largely by feedrate since the increase in feed flowrate increase the flow to the bottom.

5.2 Future Recommendation

Specify more disturbances in the model.

In the current model, the disturbance is applied only on the external flows which are feedrate, F feed composition, zF. It is recommended for the future studies to further study the responses with respect to other disturbance such as reflux, LT, boil up, VB and etc.

Solve for non constant molar flow and study the dynamic behavior.

The theory of non constant flow model has been discussed in the literature review of this report. However, due to its complexity to solve in the MATLAB and also time constrain, the method and the model developed in this report are based on constant molar flow model. As stated in the literature review, model simplification by assuming constant molar flows by neglecting energy balance is not accurate for over wide pressure application (varying P). The properties of the CDU stream can be obtained from HYSYS model which has been developed. Therefore, non-constant molar flow approaches for CDU column is recommended in the future research so that it can be discussed and compared with current model (constant molar flow) to see the deviation.

Effect of mass flows on response

Throughout this paper, the implicit assumption of all flows, L and etc., and all holdups are on a molar basis, L [kmol/min] and this assumptions is implicit in most of the distillation literature. This is the most natural choice from a modeling point of view. However, in a real column one can, at least for liquid streams, usually only adjust the mass or volumetric flows. Therefore, the responses on a real column will differ from those observed from simulations where molar flows are fixed. The reason is that a constant mass flow will result in a change in the corresponding molar flow when the composition changes. Specifically, we consider here the mass reflux L [kg/min]. [10]

The importance of using mass flows when studying real columns seems to have been appreciated only recently (Jacobsen and Skogestad, 1991). In fact, the use of mass flows may even introduce multiple steady-states and instability for columns with ideal VLE and constant molar flows [10]

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APPENDIX A

File name: crudeA.m

```
function xprime=crudeA(t,X,U)

*******************************************************************
% CRUDE DISTILLATION MODEL
% Source:(Stathis Skouras ,March 2001)
% by Nasibah Hartono
%
********************************************************************
% The model has NC*NT states
%-------------------------------------------------------------------
% ASSUMPTIONS
%-------------------------------------------------------------------
% Model assumptions:
% - NC components (multicomponent mixture); Component NC is the heavy
%   component
% - constant relative volatilities;
% - no vapor holdup;
% - constant molar flows (same vapor flow on all stages);
% - Liquid flow dynamics modelled by Franci's Weir Formula.
% - total condenser.
%-------------------------------------------------------------------
% INPUTS
%-------------------------------------------------------------------
% t    - Time in [min].
% X    - State, the first NT states are compositions of light
%        component A, the next NT states are compositions of component
B, etc,
%        compositions of the heavy component are not reported directly
%        reboiler/bottom stage is stage (1) and condenser is stage
(41).
%        The last NT states are liquid holdups in each stage.
% U(1) - Reflux L,
% U(2) - Boilup V,
% U(3) - Top or distillate product flow D,
% U(4) - Bottom product flow B,
% U(5) - Vapor side product WV,
% U(6) - Liquid side product WL,
% U(7) - feed rate F,
% U(8) - feed liquid fraction, qF.
% A   - feed compositions, zF.
% U=[U A] - Disturbances vector
% Outputs:   xprime - vector with time derivative of all the states
```

```
%----------------------------------------------------------------------
% THE MODEL
%---------------------------------------------------------------------


% Vapour-liquid equilibria(y=Kx)
y=K(1:NC-1)'*ones(1,NT).*x;



% Vapor Flows assuming constant molar flows
i=1:NT-1;     V(i)=VB*ones(1,NT-1);
i=NF:NT-1;    V(i)=V(i) + (1-qF)*F;



% Liquid flows are given by Franci's Weir Formula L(i)=K*Mow(i)^1.5
% Liquid flow L(i) dependent only on the holdup over the weir Mow(i)
% M(i)= Mow(i) + Muw(i) (Total holdup = holdup over weir + holdup
below weir)

Kuf=21.65032;                                % Constant above feed
Kbf=29.65032;                                % Constant below feed
Muw=0.25;                                    % Liquid holdup under
weir (Kmol)
i=2:NF;      L(i)= Kbf*(M(i)-Muw).^1.5;      % Liquid flows below feed
(Kmol/min)
i=NF+1:NT-1; L(i)= Kuf*(M(i)-Muw).^1.5;      % Liquid flows above feed
(Kmol/min)
L(NT)=LT;                                    % Condenser's liquid flow
(Kmol/min)

%----------------------------------------------------------------------
% Time derivatives from material balances for
% 1) Total holdup
% 2) Component holdup
%----------------------------------------------------------------------
% Column (normal stage)
j=2:NT-1;
dMdt(j) = L(j+1) - L(j) + V(j-1) - V(j);

for i=1:NC-1;
for j=2:NT-1;
dMxdt(i,j) = L(j+1)*x(i,j+1) - L(j)*x(i,j) + V(j-1)*y(i,j-1) -
V(j)*y(i,j);
end
end
```

```
% Correction for feed at the feed stage
%----------------------------------------------------------------------
% 1)The feed is assumed to be mixed into the feed stage
dMdt(NF) = dMdt(NF) + F;

dMxdt(:,NF)=dMxdt(:,NF) + F*zF(1:NC-1)';

% 2)Reboiler (assumed to be an equilibrium stage)
dMdt(1) = L(2) - V(1) - B;

i=1:NC-1;
dMxdt(i,1)= L(2)*x(i,2) - V(1)*y(i,1) - B*x(i,1);

% 3)Total condenser (no equilibrium stage)
dMdt(NT) = V(NT-1) - LT - D;

i=1:NC-1;
dMxdt(i,NT)= V(NT-1)*y(i,NT-1) - LT*x(i,NT) - D*x(i,NT);

% 4)Side product
dMdt(NP) = L(NP-1) + V(NP+1) - L(NP) - V(NP) - WL - WV;

i=1:NC-1;
dMxdt(i,NP)=L(NP-1)*x(i,NP-1) + V(NP+1)*y(i,NP+1) - L(NP)*x(i,NP) -
V(NP)*y(i,NP) - WL*x(i,NP) - WV*y(i,NP);

% Compute the derivative for the mole fractions from
%                    d(Mx) = x dM + M dx
dxdt=(dMxdt-x.*(ones(NC-1,1)*dMdt))./(ones(NC-1,1)*M');

% Rearrange elements of composition vector (dxdt) for later use
Ix=[1:(NC-1)*NT]';
W=dxdt';
dxdt=W(Ix);

% Output
xprime=[dxdt;dMdt'];
```

File Name:crudeA_lv.m

```
function xprime=crudeA_lv(t,X)
% sample usage:
[t,x]=ode15s('crudeA_lv',[0 20000],0.5*ones(1,NC*NT));
% keep record of results: lengthx=size(x); Xss=x(lengthx(1),:)';

%           Inputs are reflux (LT) and boilup (VB). Disturbances
%           are feedrate and feed composition. These are set by %
            directly altering 'crudeA_lv.m'. Outputs are liquid %
            compositions
%           for light and intermediate components and
%           liquid hold up for stages 1 through NT, given in x

% Number of stages in the column
NT=38;

%Number of components
NC=6;

% Inputs and disturbances
LT=2.70629;                          % Reflux
VB=3.20629;                          % Boilup
WV=0.00;                             % Vapor Side Prod
WL=0.00;                             % Liquid Side Prod
F=1.0 + 0;                           % Feedrate
qF=1.0;                              % Feed liquid fraction

zF=[0.01 0.45 0.113 0.18 0.03 0.22]; % Feed compositions for crude A
to component NC


% P-Controllers for control of reboiler and condenser hold up.
KcB=10;  KcD=10;                     % controller gains
MDs=0.5; MBs=0.5;                    % Nominal holdups - these are
rather small
Ds=0.5; Bs=0.5;                      % Nominal flows
MB=X((NC-1)*NT+1);  MD=X(NC*NT);     % Actual reboiler and condenser
holdup
D=Ds+(MD-MDs)*KcD;                   % Distillate flow
B=Bs+(MB-MBs)*KcB;                   % Bottoms flow

% Store all inputs and disturbances
U(1)=LT; U(2)=VB; U(3)=D; U(4)=B; U(5)=WV; U(6)=WL; U(7)=F; U(8)=qF;
A=zF; U=[U A];

xprime=crudeA(t,X,U)
```

File Name: crude4_F1.m

```
function xprime=crude4(t,X)
% sample usage:   [t,x]=ode15s('crude4',[0 20000],0.5*ones(1,NC*NT));
% keep record of results: lengthx=size(x); Xss=x(lengthx(1),:)';

%            Inputs are reflux (LT), boilup (VB), distillate (D) and %
             bottoms (B)
%            Disturbances are feedrate and feed composition.
%            These are set by directly altering 'crude4.m'.


% Inputs and disturbances
LT=2.70629;                            % Reflux
VB=3.20629;                            % Boilup
WV=0;                                  % Vapor Side Prod
WL=0;                                  % Liquid Side Prod
D=0.5;                                 % Distillate
B=0.5;                                 % Bottoms
F=10.0 + 0.1;                           % Feedrate
qF=1.0;                                % Feed liquid fraction

zF=[0.01 0.45 0.113 0.18 0.033 0.22];  % Feed compositions for
component A to component NC

% Store all inputs and disturbances
U(1)=LT; U(2)=VB; U(3)=D; U(4)=B; U(5)=WV; U(6)=WL; U(7)=F; U(8)=qF;
A=zF; U=[U A];

xprime=crudeA(t,X,U);
```

File Name:running_crudeA.m

```
%runnning distillation model 'crudeA' for any mixture of NC components
clear all
[t,x]=ode15s ('crudeA_lv',[0 300],0.5*ones(1,6*38));
lengthx=size(x);
% Vector 'Xss' returns the steady-state molar compositions of
components 1 to NC-1 at all NC stages and molar liquid holdups at all
NC stages
Xss=x(lengthx(1),:)';

save crudeA_ss  % saves in crudeA_ss.m
```

File Name:plotcrude.m

```
[t,x]=ode15s('crude4_F1',[0 300],Xss);
t0 = t; M1=x(:,39); xB = x(:,1); xD = x(:,38); % Save the data for
plotting

xprofile=Xss(1:38);

disp('Finished. Plot MB, xB and yD as a function of time.....');
% Plot reboiler holdup (Apparent delay of about 1.26 min)
figure(1); plot(t0,M1); title('MB (Kmol/min) vs t(min): Reboiler
Holdup Versus Time')
figure(2); plot(t0,xB); title('xB vs t: Reboiler Composition')
figure(3); plot(t0,xD); title('xD vs t: Distillate Composition')
figure(4);plot(x);
figure(6);plot(xprofile);title('xprofile: light composition from
bottom to top ')
figure(7);plot(t,x);
```