Dynamic Simulation of High Purity

Distillation Column

by

Abdullah Baihaqi Adzha bin Zubir

Dissertation submitted in partial fulfilment of

the requirements for the

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CERTIFICATION OF APPROVAL

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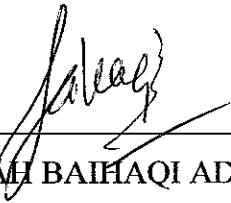(CHEMICAL ENGINEERING)

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UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK

JUNE 2009

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.

(ABDULLAH BAIHAQI ADZHA BIN ZUBIR)

ABSTRACT

This report presents a research study on dynamic simulation of high purity distillation column via MATLAB. The dynamic nature and the nonlinear behaviour of distillation equipment pose challenging control system design when products of constant purity are to be recovered. Several alternative column configurations and operating policies have been studied. However, issues related to the online operation of such process have not been properly addressed. The present work describes the investigation with experimental verification of computer based control strategies to distillation. The scope of work for the project is to conduct a literature review on dynamic behaviour of high purity distillation column The study provides a method of studying the dynamic behaviour of column comprising the steps of: a) generating a principle steady state and dynamic model corresponding to the distillation process; b) simulating the dynamic model for different operating condition via MATLAB; c) Develop output trend towards changes in input via Pseudo Random Binary Sequence (PRBS); e) Develop step response of first order process ; and f) obtain the gain and time constant for any changes of column operating condition through first order process response for control purposes A distillation model with 41-stage column with the overhead condenser as stage 1, the feed tray as stage 21 and the reboiler as stage 41 is used. The findings show that the models represent an ideal distillation column. All the research and findings obtained will be used to improve the overall performance of the column as well as to improve the quality of the product and maximise profitability. The successful outcome of this project will be a great helping hand for industrial application.

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

The process industries are dynamic. Dynamic in that process plants rarely run at a steady state condition. Feed and environmental disturbances, changes in ambient conditions, equipment vibrations, heat exchanger fouling and degrading equipment performance continually affect the smooth running of a process operation. The transient behavior of the process system is studied using a lot of dynamic simulation tools like PROII, ICON, HYSYS™ and mathematical modeling tools like MATLAB, GAMS and LINDO. Mathematical models represent sets of equations that mathematically describe the process. The term "simulator" refers to a computer program or a digital system running a computer program that implements the mathematical model.

Through dynamic simulation and mathematical modeling, analyses users are able to effectively study the impacts that changing operating conditions and design modifications have on the operation of a process. Process configurations and control system designs can be evaluated to ensure that they will meet corporate manufacturing objectives regardless of changing process and market conditions. The design and optimization of a chemical process involves the study of both steady state and dynamic behavior. Steady state models can perform steady state energy and material balances and evaluate different plant scenarios. The design engineer can use steady state simulation to optimize the process by reducing capital and equipment costs while maximizing production. Dynamic models allow the design engineer to design and compare alternative control strategies, examine the dynamic response to system disturbances and optimize the tuning of controllers in order to improve the overall performance of the plant.

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1.2   Problem Statement

Distillation is the most frequently used separation process. It separates the components of a mixture on the basis of their boiling points and on the difference in the compositions of the liquids and their vapors.

Certain types of distillation columns are designed to produce high purity and ultra purity products that is product having purity greater than approximately 99.99% by volume. Such columns are particularly sensitive to the liquid/vapor ratio and can exhibit multiple steady=state temperature profiles that will rapidly change from one profile to one profile based on the amount of vapor rising in the column and the amount of heat introduced into the column. As a result, during upset condition caused by changed in feed composition, it can be difficult, to control the liquid vapor ratio within the column and therefore the product quality.

The product purity of a distillation process is only can be maintained by the manipulation of the material and energy balances. Difficulties in maintaining that purity arise because of dead times, nonlinearities and variable interactions.

1.3   Objectives

The project is mainly about modeling a steady state and dynamic simulation for the high purity distillation column via MATLAB. Upon completing the project, a few objectives need to be achieved. The objectives of the study are as follows:

i.   To study behavior of high purity distillation column at steady state and dynamic condition.

ii.   To develop steady state and dynamic model of high purity distillation column via MATLAB.

iii. To investigate effect of reflux and reboiler rate disturbance towards top and bottom product purity.

iv. To obtain the gain and time constant for any changes of column operating condition through first order process response

1.4 Scope of Work

The scope of work for the project is to conduct a literature review on dynamic behavior of high purity distillation column. The next step is to proceed with developing mathematical model of distillation, come out with findings on effect of disturbance changes towards product purity and also obtaining gain and time constant in order to develop first order response of top and bottom product when column operating condition changes. Through this project student is exposed to explore research problems and build research objectives, applying appropriate methodology, analyzing and interpreting data obtained from the mathematical modeling, troubleshooting any predicaments occur and also reporting the findings.

CHAPTER 2

LITERATURE REVIEW AND THEORY

2.1 Distillation Process

Distillation column is probably the most popular and important process studied in the chemical engineering literature. Distillation is used in many chemical processes for separating feed streams and for purification of final and intermediate product streams. Most columns handle multicomponent feeds. But many can be approximated by binary or pseudobinary mixtures.

Distillation can be performed either as a batch or a continuous operation. The main difference between the two is that in continuous distillation, the feed concentration is relatively constant, while in batch, the concentration of the light components drops and that of the heavy components rises as distillation progresses.

Another basic difference between distillation operations is in the handling of the heat removed by the condenser at the top of the column. The more common approach is to waste that heat by rejecting it into the cooling water. In this case, "pay heat" must be used at the bottom of the column in the reboiler. Figure 2.1 illustrates this configuration and identifies its main components. Because a large part of the total operating cost is in providing the heat required at the reboiler in some distillation systems, the heat content of the bottom product is used to preheat the feed to the column.
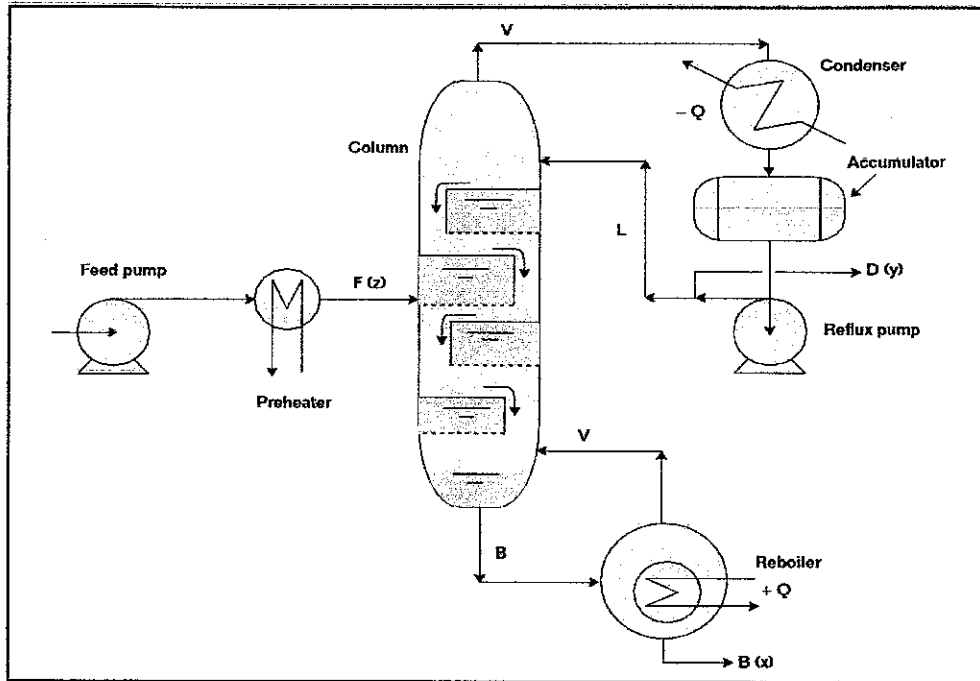
Figure 2.1: Illustration of a tray-type distillation tower, where
(without accumulation), the material balance is
F = D + B and D = V − L.

The mole fractions of the light key component in the bottoms, distillate and feed are identified as x, y and z. For binary separation, $S = (y[1-x])/(x[1-y])$.

The other option is to recycle the heat removed at the condenser by a heat pump (compressor). In this configuration, as the vapors from the column (V) are condensed, the heat from the condenser is used to vaporize a working fluid. These vapors are at the low pressure of the suction side of the compressor (heat pump). When the working fluid vapors are compressed, and these high-pressure (and temperature) vapors in the reboiler contact the bottoms liquid from the column, they condense, and their heat of condensation serves to vaporize the liquid from the column bottoms (Figure 2.2). While vapor recompression is energy-efficient, it is not used very frequently.
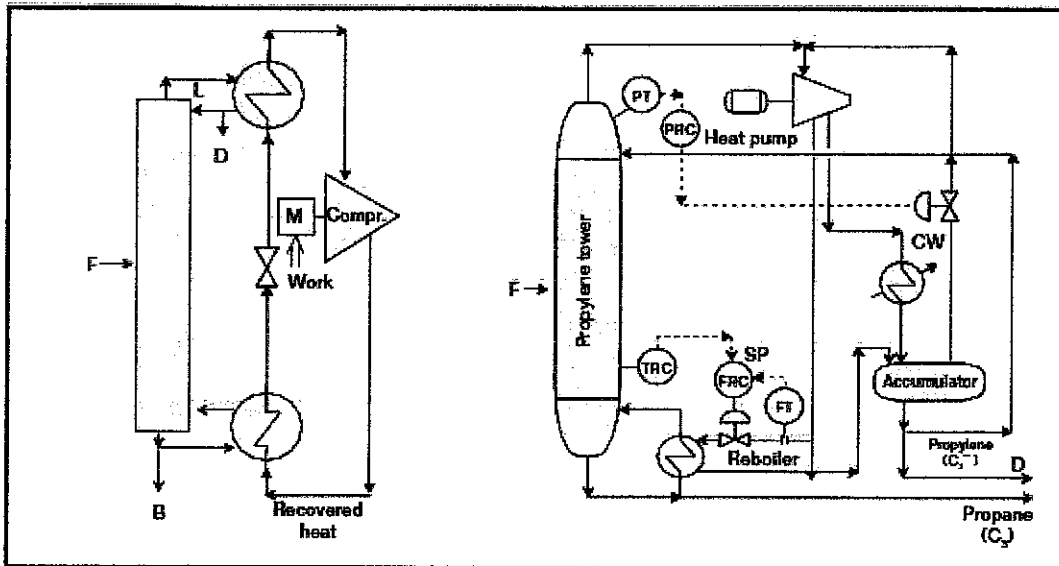
Figure 2.2: Left   : The vapor recompression system uses recovered heat.
Right : The pressure of such a distillation process can be
controlled by modulating the speed of the compressor
or by throttling the bypass around it.

2.2   The Column

The main distillation equipment is the *column, tower or fractionator*. It has two
purposes: First, it separates a feed into a vapor portion that ascends the column and a
liquid portion that descends; second, it achieves intimate mixing between the two
counter-current flowing phases. The purpose of the mixing is to get an effective transfer
of the more volatile components into the ascending vapor and a corresponding transfer
of the less volatile components into the descending liquid.

The separation of phases is accomplished by the differences in vapor pressures, with the
lighter vapor rising to the top of the column and the heavier liquid flowing to the bottom.
The portion of the column above the feed is called the *rectifying* section and below the
feed, the *stripping* section. The intimate mixing is obtained by either filling the column
with lumps of an inert material (*packing*) or by the use a number of horizontal plates, or

trays, which cause the ascending vapor to bubble through the descending liquid (Figure 2.3).
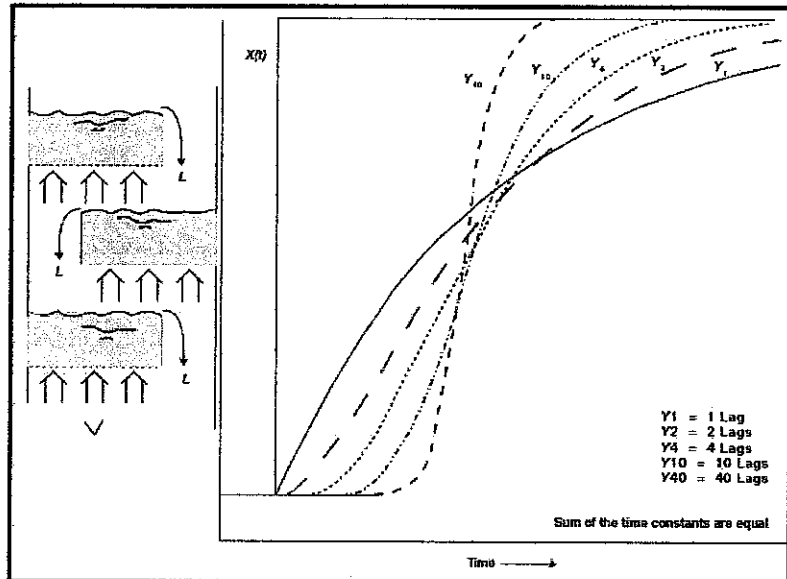
Figure 2.3: Time Lag in column tray

The contact between liquid and vapor is made intimate as the vapors ascend through the liquids held on each tray as the liquid descends is shown in the left side of Figure 2.3. The dynamics of a multiple-tray column can be approximated as a second-order lag, plus dead time.

The responses of the distillate composition (y) of 1st-, 2nd-, 4th-, 10th- and 40th-order processes are shown in the right side of Figure 2.3 which shows when a unit step change in bottoms composition (x) occurs. A 40-tray column is a 40th-order process.

Generally trays work better in applications requiring high flow, such as those encountered in high pressure distillation columns—depropanizers, debutanizers, xylene purification columns and the like. Packing works best at lower flow parameters because the low pressure drop of structured packing makes it very attractive for use in vacuum columns or ethylbenzene recycle columns of styrene plants.

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The influence of plate efficiency in the operation of the distillation tower becomes important in the control of the overhead composition. Because plate efficiencies increase with increased vapor velocities, the influence of the reflux-to-feed ratio on overhead composition becomes a nonlinear relationship.

Column dynamics are a function of the number of trays, because the liquid on each tray must overflow its weir and work its way down the column; therefore, a change in composition will not be seen at the bottom of the tower until some time has passed. These lags are cumulative as the liquid passes each tray on its way down the column. Thus, a 30-tray column could be approximated by 30 first-order exponential lags in a series of approximately the same time constant. The effect of increasing the number of lags in series is to increase the apparent dead time and increase the response-curve slope. Thus, the liquid traffic within the distillation process is often approximated by a second-order lag, plus dead time (Figure 2.3, right).

2.3   Column Variables and Their Pairing

Controlled variables include product compositions, column temperatures and pressure, and tower and accumulator levels. Manipulated variables include reflux, coolant, heating medium and product flows. Load and disturbance variables include feed-flow rate, feed composition, steam-header pressure, feed enthalpy, environmental conditions (e.g., rain, barometric pressure and ambient temperature) and coolant temperature.

The general guidelines for pairing manipulated variables with controlled variables are as follows:
- Manipulate the stream that has the greatest influence on the controlled variable.
- Manipulate the stream that is more nearly linear with the controlled variable.
- Manipulate the stream that is least sensitive to ambient conditions.

- Manipulate the stream least likely to cause interaction.

In a binary distillation process, the number of independent variables is eleven, and the number of defining equations is two. Therefore, the number of degrees of freedom is nine. Consequently, the maximum theoretical number of automatic controllers that can be used on a binary distillation process is nine, but usually only five are controlled. These variables are the compositions of the bottom and top products (x and y), the levels in the column base and accumulator, and the column pressure. The manipulated variables that can be assigned to control these are the distillate (D), bottoms (B) and reflux (L) flows, the vapor boil-up (V set by heat input QB), heat removal (QT) and the ratios of L/D or V/B. These five single loops can theoretically be configured in 120 different combinations, and selecting the right one is a prerequisite to stability and efficiency.

Column pressure almost always is controlled by heat removal (QT). This loop closes the heat balance around the column, while the levels are controlled to close its material balance. Therefore, the key task is the assignment of the manipulated variables to the composition controllers. No matter how we make that selection, these two loops will interact. A change in one will upset the other because whenever the openings of their control valves change, the material and heat balance of the column will also change.

Therefore, the most important decision in designing the distillation controls is to assign the least-interacting manipulated variables to the composition control loops. The tool used in making that selection is the relative gain (RG) calculation.

2.4   Composition Control

Conceptually, product quality is determined by the heat balance of the column. The heat removal determines the internal reflux flow rate, while the heat addition determines the internal vapor rate. These internal vapor and liquid flow rates determine the circulation rate, which in turn determines the degree of separation between two key components.

The first task in configuring the control system for a distillation column is to configure the primary composition control loops. This configuration must consider the interaction between the proposed control loops, the column's operating objectives and the most likely disturbance variables. The measurements of the composition control loops can either be direct or inferred. Table 2.1 provides some guidance on how to select the manipulated variables for controlling the compositions (and levels) of distillation columns.

Table 2.1: Sensitivity Limitations on the Paring of Distillation Control Variables

Controlled Variables \ Manipulated Variables	Distillate Flow (D)	Bottoms Product Flow (B)	Vaporization Rate (V) or Heat Input at Reboiler (Q)	Reflux Flow Rate (L)
Composition of Overhead Product (y)	OK if L/D ≥ 6 Note 3		Notes 1 and 2	Note 2
Composition of Bottoms Product (x)		Note 3	Notes 1 and 2	OK if trays ≤ 20
Accumulator Level	OK if L/D ≤ 6		Not good with furnace. OK if V/B ≥ 3	OK if L/D ≥ 0.5
Bottoms Level		OK if V/B ≤ 3	Not good if furnace is used. OK if diameter at bottom ≤ 20 ft.	

Notes:

1. Controls the concentration (x or y) which has the shorter residence time by throttling vapor flow (v).

2. More pure product should control separation (energy).

3. Less pure product should control material balance.

4. When controlling both x and y, the only choices for possible pairings are

a. Control y by D and x by V,

b. Control y by D and x by L,

c. Control y by L and x by V,

d. Control y by B and x by L.

Of these choices, d is not recommended because a y/B combination is not responsive dynamically.

2.5 Dynamic Modelling

Dynamic models are used to predict how a process and its controls respond to various upsets as a function of time. They can be used to evaluate equipment configurations and control schemes and to determine the reliability and safety of a design before capital is committed to the project. For grassroots and revamp projects, dynamic simulation can be used to accurately assess transient conditions that determine process design temperatures and pressures. In many cases, unnecessary capital expenditures can be avoided using dynamic simulation.

Dynamic simulation during process design leads to benefits during plant start-up. Expensive field changes, which impact schedule, can often be minimized if the equipment and control system is validated using dynamic simulation. Start-up and shutdown sequences can be tested using dynamic simulation.

Dynamic simulation also provides controller-tuning parameters for use during start-up. In many cases, accurate controller settings can prevent expensive shutdowns and accelerate plant start-up. Dynamic simulation models used for process design are not based on transfer functions as normally found in operator training simulators, but on fundamental engineering principles and actual physical equations governing the process. When used for process design, dynamic simulation models include:

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- Equipment models that include mass and energy inventory from differential balances
- Rigorous thermodynamics based on property correlations, equations of state, and steam tables
- Actual piping, valve, distillation tray, and equipment hydraulics for incompressible, compressible, and critical flow

These models are so detailed that the results can influence engineering design decisions and ensure a realistic prediction of the process and the control system's interaction to assess control system stability.

CHAPTER 3

METHODOLOGY

The design procedure that provides a method of controlling a process comprising the steps of:

Step 1   Generating a principle steady state and dynamic model corresponding to the distillation process

Step 2   Simulating the dynamic model for different operating condition via MATLAB

Step 3   Develop output trend towards changes in input via Pseudo Random Binary Sequence (PRBS)

Step 4   Develop step response of first order process

Step 5   Obtain the gain and time constant for any changes of column operating condition through first order process response for control purposes

3.1   Generating a Principle of Steady State and Dynamic Model Corresponding to the Distillation Process

In this section is derivation of a linearized model of the plant. Separation of input components, the feed, is achieved by controlling the transfer of components between the various stages (also called trays or plates), within the column, so as to produce output products at the bottom and at the top of the column.

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In a typical distillation system (Figure 3.1), two recycle streams are returned to the column. A condenser is added at the top of the column and a fraction of the overhead vapor V is condensed to form a liquid recycle L. The liquid recycle provides the liquid stream needed in the tower. The remaining fraction of V is the distillate- or top product. A vaporizer or reboiler is added to the bottom of the column and a portion of the bottom liquid, Lb, is vaporized and recycled to the tower as a vapor stream Vb. This provides the vapor stream needed in the tower, while the remaining portion of Lb is the bottom product.

The stages above the feed stage (index i < nf) define the enriching section and those below the feed stage (index i > nf) the stripping section of the column. The material balance equations for the feed stage and the stages in the stripping section of the column are affected by the continuous feed to the column and the withdrawal of the bottom product from the reboiler.
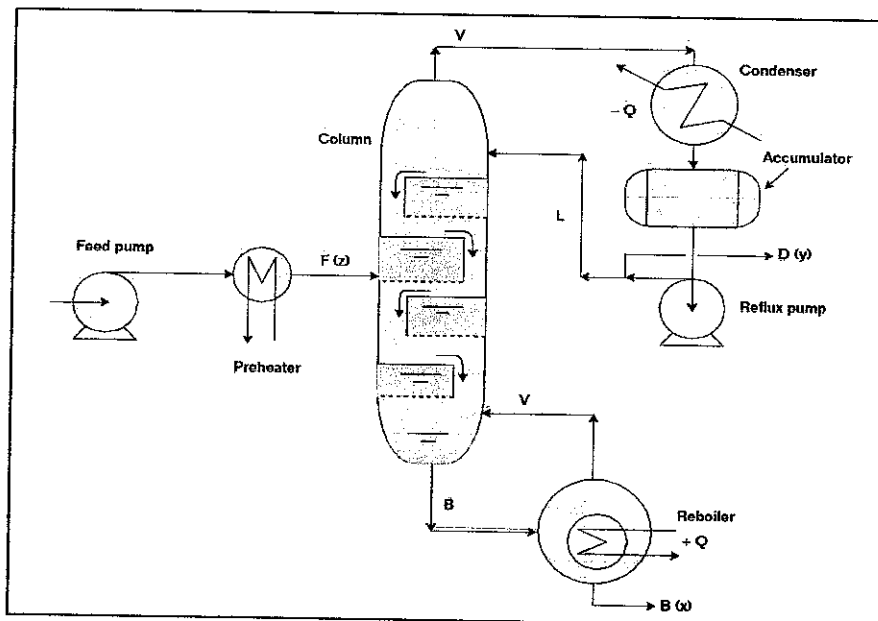

Figure 3.1 Typical distillation column

Figure 3.2 :Conceptual material balance diagram for a typical stage.

Figure 3.3 :Conceptual material balance diagram for the feed stage.
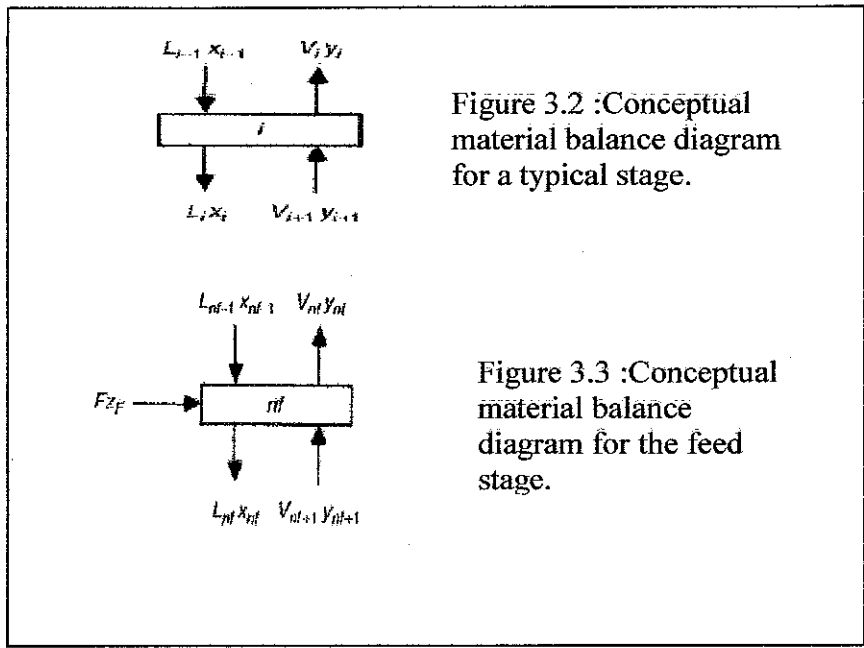
Table 3.1 : Mass and Component Balance on Distillation Column

Overall Balance	$F = D + B$
Overall Component Balances	$Fzf = Dxd + Bxb$
Condenser Balance	$V = Lr + D$
Reboiler Balance	$Vb = Ls - B$
Feed Balance	$V_{NF} = V_{NF+1} + F(1 - q_F)$ $L_{NF} = L_{NF-1} + Fq_F$
Feed Stage Balance	$\dfrac{dx_{NF}}{dt} = \dfrac{1}{M_T} [L_R x_{NF-1} + V_S y_{NF+1} + Fz_F - L_S x_{NF} - V_R y_{NF}]$
All Stages Except Feed, Condenser, and Reboiler	$\dfrac{dx_i}{dt} = \dfrac{1}{M_T} [L_R x_{i-1} + V_R y_{i+1} - L_R x_i - V_R y_i]$

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

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composition zF [molefraction]. L [kmole/hr] denotes the reflux flow rate of the condenser, Vb [kmole/hr] is the boilup flow rate of the reboiler. The variable

$$u = \begin{pmatrix} L \\ V_b \\ F \end{pmatrix}$$

(3-1)

is taken as input of the plant. The top product consists of a distillate stream D [kmol/hr], with composition Xd [mole fraction]. Likewise, the bottom product consists of a bottom stream B, with composition XB [mole fraction]. The output of the system is taken to be

$$y = \begin{pmatrix} X_d \\ X_b \end{pmatrix}$$

(3-2)

It is assumed that the vapor leaving a stage is in equilibrium with the liquid on the stage. The relationship between the liquid and vapor phase concentrations on a particular stage can be calculated using the constant relative volatility expression in Eq. (3-3).

$$y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i}$$

(3-3)

3.2 Simulating the Dynamic Model for Different Operating Condition via MATLAB

In order to simulate the dynamic model, it is needed to solve the steady state equation. First, obtained the steady-state concentrations by solving the system of equations, $f(x) \approx 0$.

From the overhead receiver component balance:

$$f_1 = y_2 - x_1 = 0 \tag{3-4}$$

From the rectifying section component balance ($i = 2$ to NF-1):

$$f_i = L_R x_{i-1} + V_R y_{i+1} - L_R x_i - V_R y_i = 0 \tag{3-5}$$

From the feed stage balance:

$$f_{NF} = L_R x_{NF-1} + V_S y_{NF+1} + F z_F - L_S x_{NF} - V_R y_{NF} = 0 \tag{3-6}$$

From the stripping section component balance ($i=$ NF+ 1 to NS-1):

$$f_i = L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i = 0 \tag{3-7}$$

And from the reboiler component balance:

$$f_{NS} = L_S x_{NS-1} - B x_{NS} - V_S y_{NS} = 0$$

where $B = Ls - Vs.$

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It is realize that the all the equations to solve steady state constitute a set of nonlinear algebraic equations, since the relative volatility relationship equation is nonlinear in the state variable.

The equations arc *NS* equations in *NS unknowns*. A Newton-based technique will be used to solve the equations.

3. 3   Output Trend Towards Changes in Input via Pseudo Random Binary Sequence (PRBS)

By using a simulink, a multiple step change of input can be done by using PRBS.The purpose is to determine the trend of output response towards changes in input.
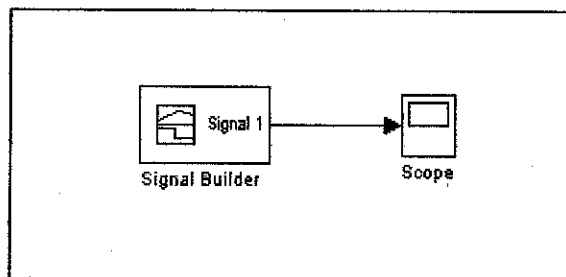

Figure 3.2: Model of input via Simulink

The use of signal builder is to create and generate interchangeable groups of signals whose waveforms are piecewise linear. Type of signal is set as PRBS with frequency of 10.

3.4 Response of First Order Process

First Order Process is use to find how the outlet composition changes when either of the inputs, reflux (R) or reboiler rate (Vb) is changed. Here is the general first-order transfer function,

$$G_p(s) = \frac{Y(s)}{U(s)} = \frac{K_p}{\tau_p s + 1} \tag{3-9}$$

where K_p : process gain

τ : time constant

$U(s)$: input

$Y(s)$: output

3.5 Step Response of First Order Process

For a step input of magnitude M, $U(s) = M/s$, and (1-1) becomes

$$Y(s) = \frac{K_p M}{s(\tau_p s + 1)} \tag{3-10}$$

By Laplace transform, the time domain response is

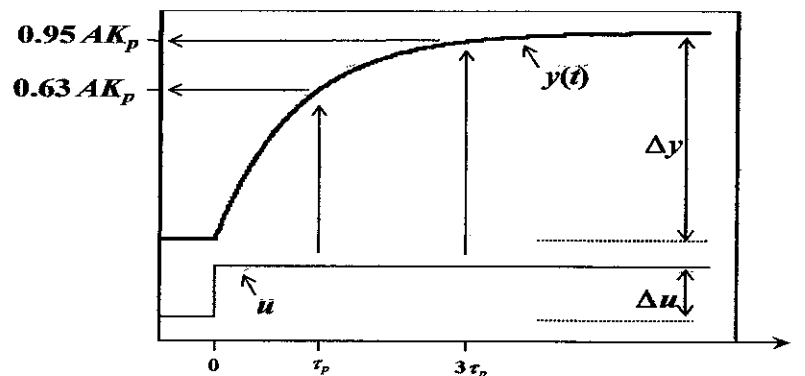$$y(t) = K_p M (1 - e^{-t/\tau_p}) \tag{3-11}$$

Figure 3.3: Step response of first-order process

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The plot of equation shows that a first-order process does not respond instantaneously to a sudden change in its input. In fact, after the time interval equal to the process time constant (t= τ), the process response is still only 63.2% complete. Theoretically, the process output never reaches the new steady state value except as t → ∞; it does approximate the final steady-state value. Notice that Figure 3.5 has been drawn in dimensionless or normalized form, with time divided with process time constant and the output change divided by the product of the process gain and magnitude of the input change.

CHAPTER 4

RESULT AND DISCUSSION

4.1   Steady State Operation of a 41-Stage Column

Consider a 41-stage column with the overhead condenser as stage 1, the feed tray as stage 21 and the reboiler as stage 41. The following parameters and inputs apply:

α = 1.5

F = 1 mol/min

z_F = 0.5 mole fraction of light component

R = 2.706 mol/min

D = 0.5 mol/min

q_F = 1 (sat'd liquid)

From an overall material balance, the bottoms product flowrate is;

$$B = F - D = 1 - 0.5 \text{ mol/min}$$

the stripping section flowrate is:

$$L_s = R + Fq_F = 2.706 + 1 = 3.705 \text{ mol/min}$$

and a balance around the reboiler yields:

$$V_s = L_s - B = 3.706 - 0.5 = 3.206 \text{ mol/min}$$

The **m-file dist_ss.m** (shown in the Appendix) is used to solve for the steady-state compositions.

The resulting compositions are shown in Figure 4.1. The sensitivity to reflux rate and reboiler rate is also shown by the plot in Figure 4.2 and Figure 4.3.

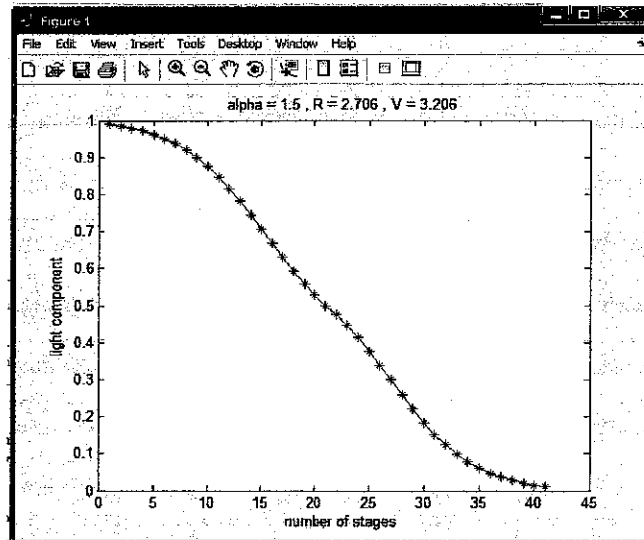21

Figure 4.1 Liquid phase composition (mol fraction of light component) as a function of stage number

Figure 4.1 above shows the steady state profile of a distillation column at fixed reflux and vapor reboiler rate. So as the number of stages increases (towards reboiler), less light component are recovered.
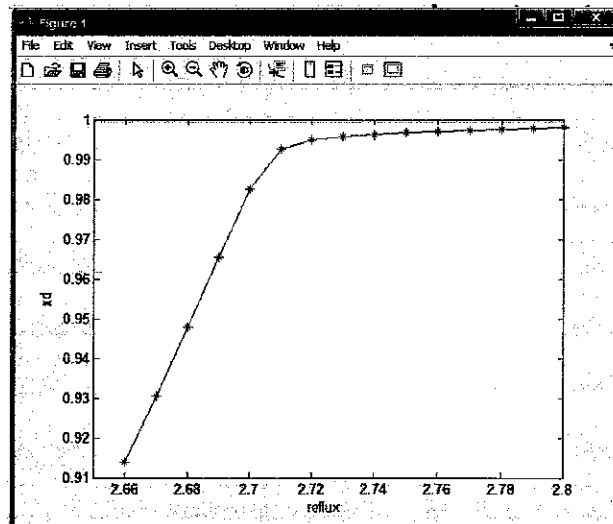

Figure 4.2 Steady-state input (reflux) output (distillate composition) relationship

From Figure 4.2 above, the steady-state gain (change in output/change in input) for distillate composition is large when reflux is less than 2.7, but small when the reflux is greater than 2.71 mol/min.
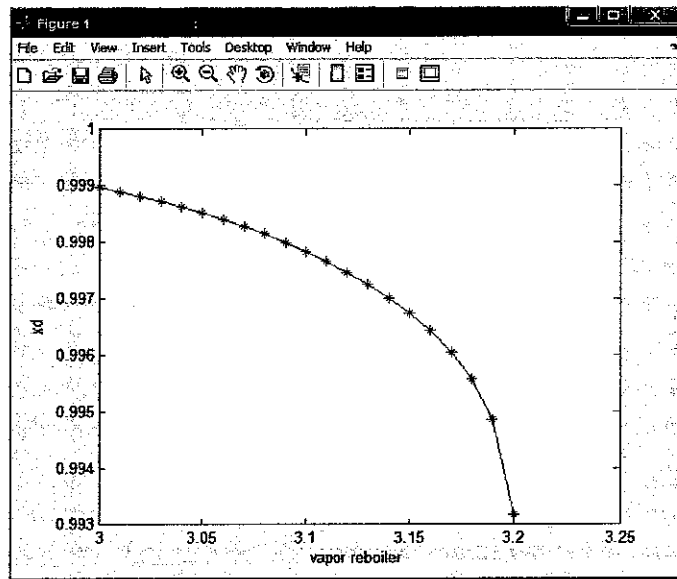
Figure 4.3 Steady-state input (vapor reboiler) output (distillate composition) relationship

From Figure 4.3 above, by varying vapor boil up flow rate, the steady-state gain (change in output/change in input) for distillate composition is large when vapor boil up flow rate is greater than 3.15 and small when less than 3.15 mol/min.

So, by this two variables, reflux and vapor boil up flow rate operating condition will have great influence on distillate and bottom product purity .This sensitivity has important implication for control design system.

4.2   Dynamic Operation of a 41-Stage Column

Consider now the previous problem, with the initial conditions of the stage compositions equal to the steady-state solution. The additional parameters needed for the dynamic simulation are the molar holdups on each stage. Here we use the following parameters:

M_1 = Md =   overhead receiver molar holdup   = 5 mol

M_2 =   tray molar holdup   = 0.5 mol

M_3 =   hottoms (reboiler) molar holdup   = 5 mol

The nonlinear behavior of distillation column are illustrated and the result of ±1 step changes in the reflux and vapor reboiler rate at t= 5 minutes are compared. Refer Figure 4.4 and Figure 4.5 below.
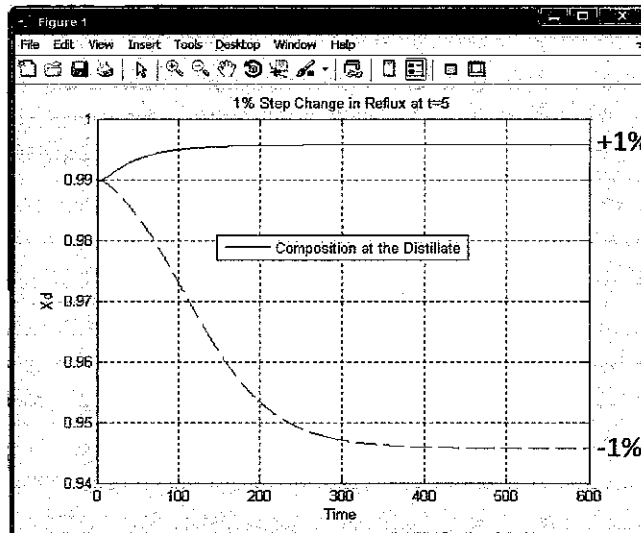
Figure 4.4 Disturbance of ±1 step change in reflux rate

As seen from Figure 4.4, the dynamic state model follows the steady state model in its trends to changes in the reflux flow rate. The step disturbance of +1% to the reflux flow rate produces a top product that is almost 100% pure. In the mean time, a

-1% step disturbance to the reflux flow rate results in top product being only slightly above 94% purity.
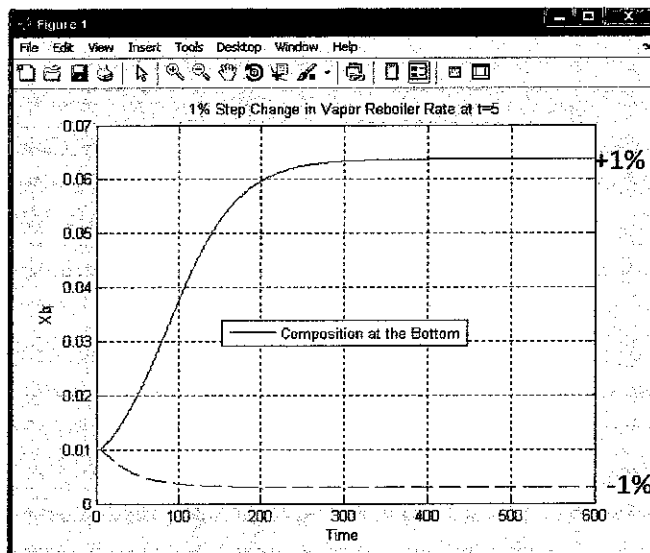
Figure 4.5 Disturbance of ±1 step change in vapor reboiler rate

From Figure 4.5, as reboiler vapor flow rate is increased, more of the bottom product (heavier component) is vaporized hence reduced top product purity. However, reduction of 1% vapor reboiler rate ensures almost 99% recovery of heavy component at the bottom.

4.3 Output Trend towards Changes in Input via Pseudo Random Binary Sequence (PRBS)

By using a simulink, a multiple step change of input is done by using PRBS. Type of signal is set as PRBS with frequency of 10.
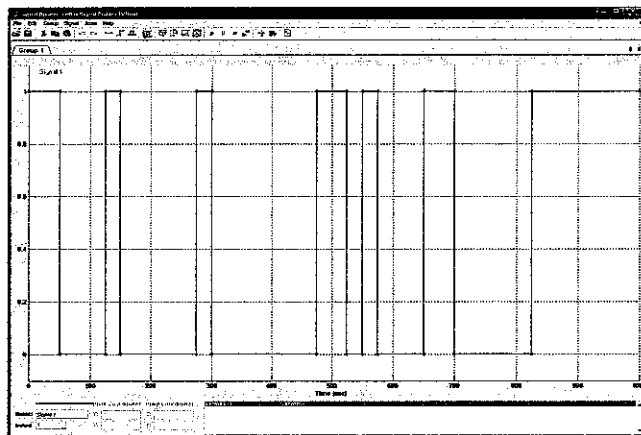
Figure 4.6: ±1% changes of reflux via PRBS at frequency = 10

Figure 4.6 shows the series of ±1% step changes of reflux at frequency 10 via PRBS. The result from the changes of reflux towards distillate is shown in Figure 4.7.
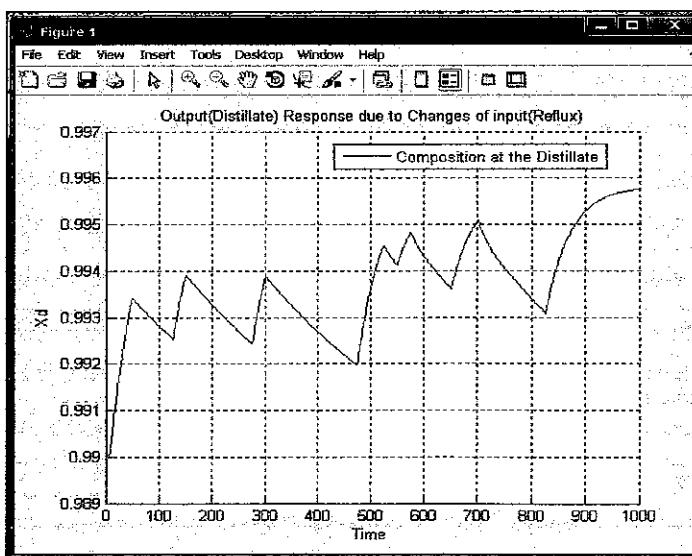
Figure 4.7: Trend of distillate response towards changes in reflux via PRBS

From Figure 4.7, we see that every step change of reflux will affect the distillate response.+1% step change of reflux, lead to higher distillate purity while =1% step change of reflux only lead to loss of product purity. Higher amount of reflux introduced to the distillation will lead to high top product purity due to more mass transfer occurred between reflux liquid and vapor from reboiler.

Figure 4.8: ±1% changes of reboiler vapor rate via PRBS at frequency = 10

Figure 4.8 shows the series of ±1% step changes of reboiler vapor rate at frequency 10 via PRBS.The result from the changes of reboiler vapor rate toward bottom purity is shown in Figure 4.9.
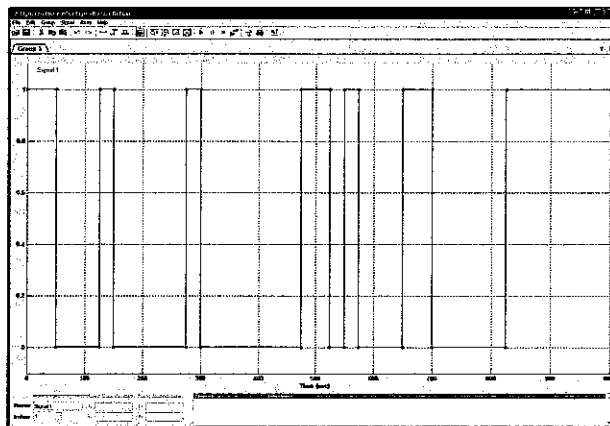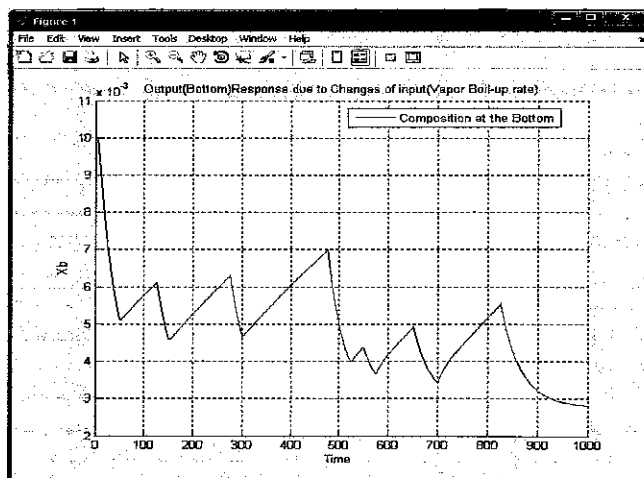

Figure 4.9: Trend of bottom response towards changes in reboiler vapor rate via PRBS

From Figure 4.9, we see that every step change of reboiler vapor rate will affect the bottom response.+1% step change of reboiler vapor rate, lead to lower bottom product purity while -1% step change of reboiler vapor rate leads to increase of product purity. As more reboiler rate is introduced in the column, there will be lesser product purity escaped at the bottom hence increase product recovery at the top. Less reboiler vapor rate will cause deficiency of stripping of light component.

4.4   Step Response of First Order Process

Below are the step responses by top product, xd and bottom product, xb gain with respect to changes of reflux ,Δu.

Figure 4.10: Distillate, xd gain and bottom, xb gain response with respect to changes of reflux , Δu.

Figure 4.10 shows that the gain for distillate, xd and bottom, xb is increase as reflux is increase. Both gains will decrease as negative change of reflux is introduced. The gain shows the magnitude change of output response when there is change of input. The bigger the gain, the longer time needed for the distillate and bottom to reach steady state.

Table 4.1 until Table 4.4 and equations is developed from Figure 4.10

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Table 4.1 : Effect of increase of reflux towards xd

y0	yf	Δy	|Δu|	Gain K	K at 63.2%	x
0.8	0.127	-0.673	0.05412	-12.426	0.374976	0.012

$$K(u) = 0.8 - 0.673 \, (1 - e^{-u/0.012})$$

Table 4.2 : Effect of decrease of reflux towards xd

y0	yf	Δy	|Δu|	Gain K	y at 63.2%	x
0.8	1.654	0.854	0.05412	15.7748	1.339559	0.01

$$K(u) = 0.8 + 0.854 \, (1 - e^{-u/0.01})$$

Table 4.3 : Effect of increase of reflux towards xb

y0	yf	Δy	|Δu|	Gain K	y at 63.2%	x
1.029	1.665	0.636	0.05412	11.74832	1.43083756	0.01

$$K(u) = 1.029 + 0.636 \, (1 - e^{-u/0.01})$$

Table 4.4 : Effect of decrease of reflux towards xb

y0	yf	Δy	|Δu|	Gain K	y at 63.2%	x
1.029	0.142	-0.887	0.05412	-16.3844	0.4685907	0.011

$$K(u) = 1.029 - 0.887 \, (1 - e^{-u/0.011})$$
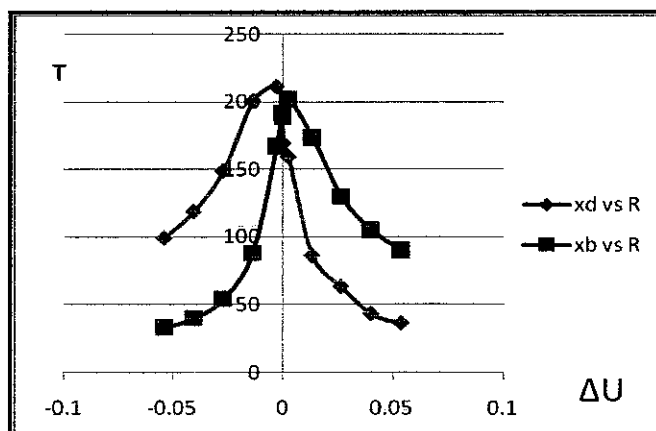
Figure 4.11: Time constant vs changes of reflux, Δu

Figure 4.11 shows that the time variation of time constant for changes of reflux. Increase of reflux leads to decrease of time constant for distillate response compared to bottom response. While decrease of reflux is vise versa. This shows that the time required for distillate to reach steady state is shorter than bottom as reflux increase. However as reflux is reduced, time required for bottom to reach steady state is shorter than distillate.

Below are the step responses by top product, *xd* and bottom product, *xb* gain with respect to changes of vapor reboiler rate ,Δu
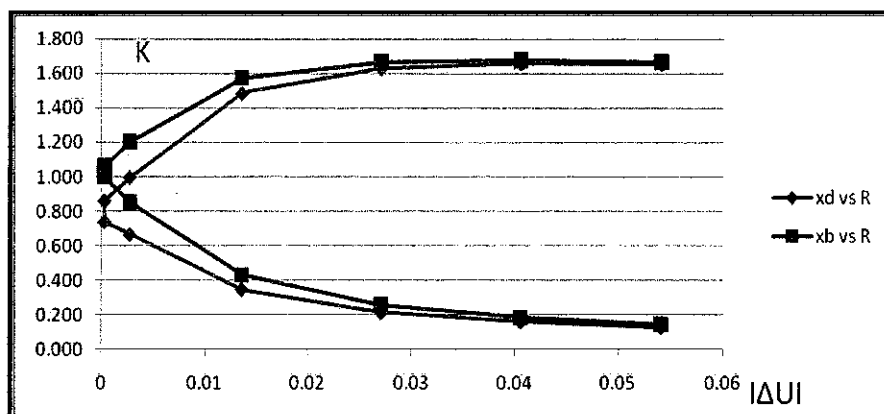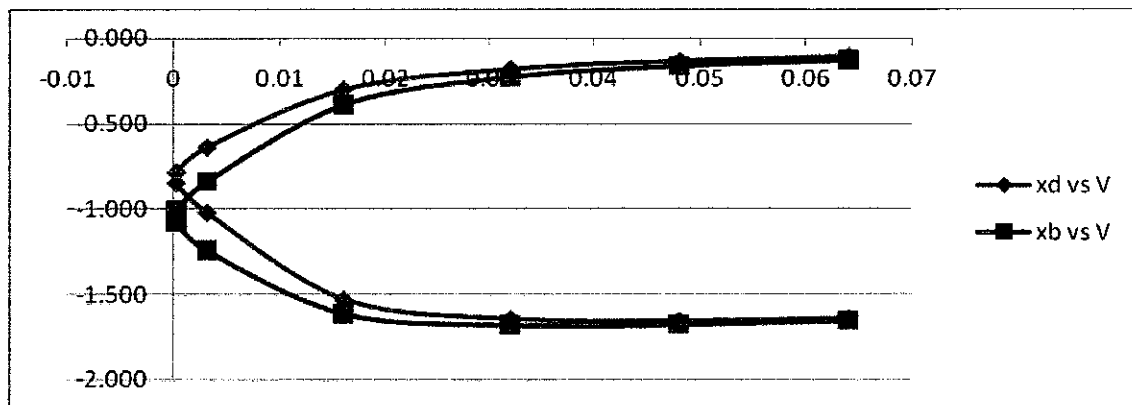

Figure 4.12: Distillate, *xd* gain and bottom, *xb* gain response with respect to changes of vapor reboiler rate, Δu.

Figure 4.12 shows that the gain for distillate, *xd* and bottom, *xb* is decrease as vapor reboiler rate is increase. Both gains will increase as negative change of reflux is introduced. The gain shows the magnitude change of output response when there is change of input. The bigger the gain, the longer time needed for the distillate and bottom to reach steady state.

Table 4.5 until Table 4.8 and equations is developed from Figure 4.12

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Table 4.5 : Effect of decrease of vapor reboiler rate towards xd

y0	yf	Δy	|Δu|	Gain,K	y at 63.2%	T
-0.817	-0.108	0.709	0.06412	11.04984	-0.3692179	0.018

$$K(t) = -0.817 + 0.709\,(1 - e^{-t/0.018})$$

Table 4.6 : Effect of increase of vapor reboiler rate towards xd

y0	yf	Δy	|Δu|	Gain,K	y at 63.2%	T
=0.817	1.63949	-0.822	0.06412	-12.827	-1.3368127	0.014

$$K(t) = -0.817 - 0.822\,(1 - e^{-t/0.014})$$

Table 4.7 : Effect of decrease of vapor reboiler rate towards xb

y0	yf	Δy	|Δu|	Gain,K	y at 63.2%	T
-1.0415	-1.653	-0.612	0.06412	-9.54353	-1.4282404	0.01

$$K(t) = -1.0415 - 1.653\,(1 - e^{-t/0.01})$$

Table 4.8 : Effect of increase of vapor reboiler rate towards xb

y0	yf	Δy	|Δu|	Gain,K	y at 63.2%	T
-1.0415	-0.126	0.915	0.06412	14.27114	-0.4631788	0.008

$$K(t) = -1.0415 + 0.915\,(1 - e^{-t/0.008})$$
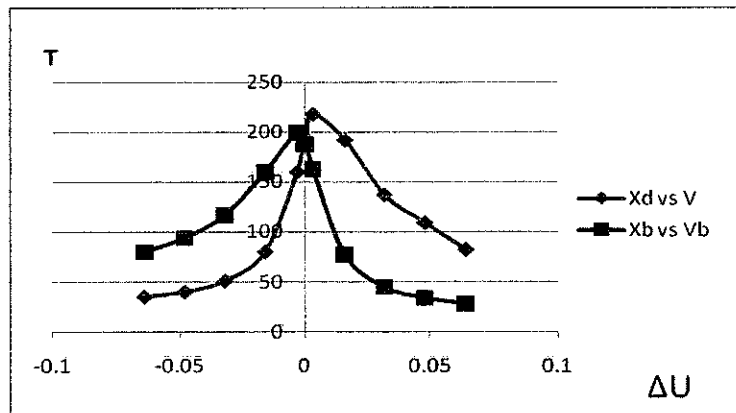
Figure 4.13: Time constant vs changes of vapor reboiler rate, Δu

Figure 4.13 shows that the time variation of time constant for changes of vapor reboiler rate. Increase of vapor reboiler rate leads to decrease of time constant for bottom response compared to distillate response. While decrease of vapor reboiler rate is vise versa. This shows that the time required for bottom to reach steady state is shorter than distillate as vapor reboiler increase. However as vapor reboiler is reduced, time required for distillate to reach steady state is shorter than the bottom.

CHAPTER 5

CONCLUSION AND RECOMMENDATION

After discussing the results of the simulations for both dynamic and steady state distillation column, it can be concluded that the objective of this project is achieved as the MATLAB models represent an ideal distillation column..The assumptions made for this project was fairly rigid and elementary. To obtain more accurate results from the simulations, the assumptions need to include:

- energy balance
- complex tray hold up
- lag time or dead time

This will ensure the model would mimic an actual behavior of distillation column.

Below are the several recommendations suggested in order to be able to pursue project further.

1. To incorporate energy balances into the mathematical model
2. To incorporate lag and dead time.
3. To incorporate the Francis Weir tray hydraulic in order to study the variation of vapor and liquid holdup
4. To incorporate a multicomponent mixture of components into the model.

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- **Steady State MATLAB Model (filename: dist_ss.m)**

dist_ss.m

```
function f = dist_ss(x)
%
 global DIST_PAR ;
 DIST_PAR =[1.5 41 21 1 0.5 1 2.706 3.206];
%
  if length(DIST_PAR) < 8;
      disp('not enough parameters given in DIST_PAR')
     disp(' ')
      disp('check to see global DIST_PAR has been defined')
      return
  end

% input
    alpha  =DIST_PAR(1);
     ns    = DIST_PAR(2);
     nf    = DIST_PAR(3);
     feed  = DIST_PAR(4);
     zfeed = DIST_PAR(5);
     qf    = DIST_PAR(6);
    reflux = DIST_PAR(7);
    vapor  = DIST_PAR(8);
%
% rectifying & stripping liquid flowrates
  lr    =  reflux;
  ls    =  reflux + feed*qf;
%
% rectifying & stripping vapor flowrates
  vs    =  vapor;
  vr    =  vs + feed*(1-qf);
%
% distilate and bottom rates
  dist  =  vr - reflux;
  lbot  =  ls - vs;
%
  if dist < 0
      disp('error in specifications, distilate flow <0')
      return
    end
    if lbot < 0
        disp('error in specifications, stripping section')
      disp(' ')
      disp('liquid flowrate is negative')
      return
    end
%
% zero function vector
  f = zeros(ns,1);
```

```
% equilibrium vapor compositions
   for i=1:ns;
       y(i)=(alpha*x(i))/(1+(alpha-1)*x(i));
   end
%
%------------------ MATERIAL BALANCES -----------------------

% overhead receiver
   f(1)=(vr*y(2)-(dist+reflux)*x(1));
%
% rectifying (top) section
   for i=2:nf-1;
       f(i)=lr*x(i-1)+vr*y(i+1)-lr*x(i)-vr*y(i);
   end
%
% feed stage
   f(nf) = lr*x(nf-1)+vs*y(nf+1)-ls*x(nf)-vr*y(nf)+feed*zfeed;
%
% stripping (bottom) section
   for i=nf+1:ns-1;
       f(i)=ls*x(i-1)+vs*y(i+1)-ls*x(i)-vs*y(i);
   end
%
% reboiler
   f(ns)=(ls*x(ns-1)-lbot*x(ns)-vs*y(ns));
```

Enter command below in Matlab command prompt after running **dist_ss.m** above.

```
>> x = fsolve('dist_ss', x0)
>> n=1:41;
>> plot(n,x, '-*')
>> title('alpha = 1.5 , R = 2.706 , V = 3.206')
>> xlabel('number of stages')
>> ylabel('light composition')
```

For simulating a relationship between distillate and variable vapor boil up rate or distillate and variable reflux rate, dist_ss.m file need to be modified as per below;

dist_ss.m

```
function f = dist_ss(x)
%
 global DIST_PAR ;
 DIST_PAR =[1.5 41 21 1 0.5 1 2.706 3.206];
```

Only this part needs to be changed.

```
              dist_ss.m   (modified)


function f = dist_A(x,R)
%
 global DIST_PAR ;
 DIST_PAR =[1.5 41 21 1 0.5 1 R 3.206];
```

Enter command below in Matlab command prompt after running modified dist_ss.m file above.

```
>> clc;
>> clear;
>> x0=0.5*ones(41,1);
>> V=[2.66:0.01:2.8];
>> n=length(R);
>> x=[];
>> for i=1:n
       a=fsolve(@(x)dist_ss(x,R(i)),x0);
       x=[x; a(1)];
end
>> plot(R,x,'-*')
>> xlabel(reflux')

>> ylabel('xd')
```

For simulating steady-state input (vapor reboiler) output (distillate composition) relationship.

```
              dist_ss.m   (modified)


function f = dist_A(x,V)
%
 global DIST_PAR ;
 DIST_PAR =[1.5 41 21 1 0.5 1 2.706 V];
```

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Enter command below in Matlab command prompt in after running modified **dist_ss.m file** above.

```
>> clc;
>> clear;
>> x0=0.5*ones(41,1);
>> V=[3:0.01:3.206];
>> n=length(V);
>> x=[];
>> for i=1:n
      a=fsolve(@(x)dist_ss(x,V(i)),x0);
      x=[x; a(1)];
end
>> plot(V,x,'-*')
>> xlabel('vapor reboiler')

>> ylabel('xd')
```

- **Dynamic MATLAB Model (filename: dist_dyn.m)**

```
function xdot = dist_dyn(t,x);
global DIST_PAR

%input
alpha   = DIST_PAR(1);   % relative volatility
ns      = DIST_PAR(2);   % total number of stages
nf      = DIST_PAR(3);   % feed stage
feedi   = DIST_PAR(4);   % initial feed flowrate
zfeedi  = DIST_PAR(5);   % initial feed composition, light comp
qf      = DIST_PAR(6);   % feed quality (1 = sat'd liqd,
%                               0 = sat'd vapor) (1)
refluxi = DIST_PAR(7);   % initial reflux flowrate
vapori  = DIST_PAR(8);   % initial reboiler vapor flowrate
md      = DIST_PAR(9);   % distillate molar hold-up
mb      = DIST_PAR(10);  % bottoms molar hold-up
mt      = DIST_PAR(11);  % stage molar hold-up
%
if length(DIST_PAR) == 19;
stepr   = DIST_PAR(12);  % magnitude step in reflux
tstepr  = DIST_PAR(13);  % time of reflux step change
stepv   = DIST_PAR(14);  % magnitude step in vapor
tstepv  = DIST_PAR(15);  % time of vapor step change
stepzf  = DIST_PAR(16);  % magnitude of feed comp change
```

```
tstepzf = DIST_PAR(17); % time of feed comp change
stepf   = DIST_PAR(18); % magnitude of feed flow change
tstepf  = DIST_PAR(19); % time of feed flow change
else

stepr = 0; tstepr = 0; stepv = 0; tstepv = 0;
stepzf = 0; tstepzf = 0; stepf = 0; tstepf = 0;
end

if t < tstepr;
reflux = refluxi;
else
reflux = refluxi + stepr;
end
%
if t < tstepv;
vapor = vapori;
else
vapor = vapori + stepv;
end
%
if t < tstepzf;
zfeed = zfeedi;
else
zfeed = zfeedi + stepzf;
end
%
if t < tstepf;
feed = feedi;
else
feed = feedi + stepf;
end

% rectifying and stripping section liquid flowrates
lr   =   reflux;
ls   =   reflux + feed*qf;

% rectifying and stripping section vapor flowrates

vs   =   vapor;
vr   =   vs +  feed*(1-qf);

% distillate and bottoms rates

dist  = vr - reflux;
lbot  =  ls - vs;

% zero the function vector
xdot = zeros(ns,1);

% calculate the equilibrium vapor compositions
for i=1:ns;
     y(i)=(alpha*x(i))/(1.+(alpha-1.)*x(i));
end
```

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```
%------------------ MATERIAL BALANCES ----------------------

% overhead receiver
xdot(1)=(1/md)*(vr*y(2)-(dist+reflux)*x(1));

% rectifying (top) section
for i=2:nf-1;
     xdot(i)=(1/mt)*(lr*x(i-1)+vr*y(i+1)-lr*x(i)-vr*y(i));
end

% feed stage
xdot(nf)  = (1/mt)*(lr*x(nf-1)+vs*y(nf+1)-ls*x(nf)-
vr*y(nf)+feed*zfeed);

% stripping (bottom) section
for i=nf+1:ns-1;
     xdot(i)=(1/mt)*(ls*x(i-1)+vs*y(i+1)-ls*x(i)-vs*y(i));
end

% reboiler
xdot(ns)=(1/mb)*(ls*x(ns-1)-lbot*x(ns)-vs*y(ns));
```

- **Dynamic State Calling File(filename: R_1p.m)**

```
%+5% step change of reflux
clc;
clear;
  global DIST_PAR
   DIST_PAR(1)=1.5;  % relative volatility (1.5)
  DIST_PAR(2)=41   % total number of stages (41)
  DIST_PAR(3)=21   % feed stage (21)
  DIST_PAR(4)=1   % initial feed flowrate (1)
  DIST_PAR(5)=0.5  % initial feed composition, light comp (0.5)
  DIST_PAR(6)=1   % feed quality (1 = sat'd liqd,
%                          0 = sat'd vapor) (1)
  DIST_PAR(7)=2.706  % initial reflux flowrate (2.706)
  DIST_PAR(8)=3.206  % initial reboiler vapor flowrate (3.206)
  DIST_PAR(9)=5   % distillate molar hold-up (5)
  DIST_PAR(10)=5 % bottoms molar hold-up (5)
 DIST_PAR(11)=0.5 % stage molar hold-up (0.5)
%
  DIST_PAR(12)=0.02706;
  DIST_PAR(13)=5;
  DIST_PAR(14)=0;
  DIST_PAR(15)=0;
  DIST_PAR(16)=0;
  DIST_PAR(17)=0;
  DIST_PAR(18)=0;
  DIST_PAR(19)=0;
```

```
x0=0.5*ones(41,1);
n=ones(41:1);
n=[1:41]';
for i=1:n
    x0=fsolve('dist_ss',x0);
end

[t,x]=ode45('dist_dyn',[0:1:600],x0);
plot(t,x(:,1)),xlabel('Time'),ylabel('Xd'),legend('Composition at the
Distillate',0)

hold on
 DIST_PAR(12)=-0.02706;
[t,x]=ode45('dist_dyn',[0:1:600],x0);
plot(t,x(:,1),'r--')
grid on
title('1% Step Change in Reflux at t=5')
```