MODELING AND SIMULATION OF A MULTICOMPONENT DISTILLATION COLUMN USING ASPEN HYSIS

A PROJECT REPORT

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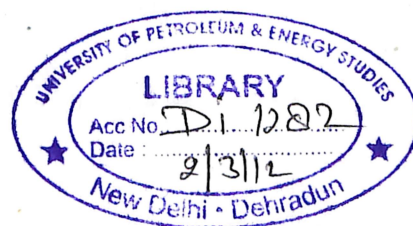Lecturer
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CERTIFICATE

This is to certify that project report on **"Modeling and Simulation of Multi-Component Distillation Column using Aspen Tech"** submitted to **University of Petroleum & Energy Studies**, Dehradun by **R. Ravin Raj and Anuroop Pandey** in partial fulfillment of the requirement of the award of degree of **Bachelor of Technology in Applied Petroleum Engineering**, session (2003-2007) is a bonafide work carried out by them under my supervision and guidance. This work has not been submitted anywhere else for any degree or diploma.

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ABSTRACT

Low cost availability of computer software and hardware, and increased computing power have led to the ever increasing computerization and automation of manufacturing operations employing chemical engineers. This trend permeates both established (chemical, petroleum) and developing (microelectronics, biotechnology) industries and has led to the significant growth of process systems engineering. Indeed, process modeling and simulation have become so accurate, fast and inexpensive so as to reduce reliance on plant scale-up. The scope of process design has been expanded to include evaluation of a large number of design alternatives from economic, safety and environmental viewpoints as well as hazard and reliability analysis. Process optimization is routinely pursued in the context of both on-line and off-line applications. Thus, process modeling and automation projects have become a major vehicle for increasing plant efficiency and abnormal situation management.

The main purpose of this project has been that we get an insight into the basics of simulating a model using a computer, which has been modeled in paper and verify the results thereafter. The objective here is to understand and correlate the theoretical model and its simulation.

Here a steady state model based on transport phenomena approach has been developed to simulate a Multi-component Distillation Unit of an operating refinery. The model uses C+3 independent variables for each stage; liquid mole fractions, total liquid flow rate, total vapor flow rate and temperature, where C is the number of components in the feed. The non-linear model equations consists of component material balances, vapor-liquid equilibrium relations, enthalpy balance and summation equations and simultaneously using a modified Newton-Raphson technique. Though the number of equations is large, due to large number of stages in the column, use of a sparse matrix technique allows a fast convergence.

After the theoretical modeling was done, it was simulated using AspenHysis. The results have been found to be satisfactory according to the referred case study.

Contents

CHAPTER 1

DISTILLTION – AN INTRODUCTION

OVERVIEW

It is the method of separating components of a solution which depends upon the distribution of substances between a gas and a liquid phase applied to cases where all the components are present in both the phases.

Distillation is based on the fact that the vapor of a boiling mixture will be richer in the components that have lower boiling points.

Therefore, when this vapor is cooled and condensed, the condensate will contain more volatile components. At the same time, the original mixture will contain more of the less volatile material.

Distillation columns are designed to achieve this separation efficiently.

Although many people have a fair idea what "distillation" means, the important aspects that seem to be missed from the manufacturing point of view are that:

- Distillation is the most common separation technique

- It consumes enormous amounts of energy, both in terms of cooling and heating requirements

- It can contribute to more than 50% of plant operating costs

TYPES OF DISTILLATION COLUMNS

There are many types of distillation columns, each designed to perform specific types of separations, and each design differs in terms of complexity. One way of classifying distillation column type is to look at how they are operated.

Thus we have:

- Batch columns

- Continuous columns.

Batch Columns

In batch operation, the feed to the column is introduced batch-wise. That is, the column is charged with a 'batch' and then the distillation process is carried out. When the desired task is achieved, a next batch of feed is introduced.

Continuous Columns

In contrast, continuous columns process a continuous feed stream. No interruptions occur unless there is a problem with the column or surrounding process units. They are capable of handling high throughputs and are the more common of the two types. We shall concentrate only on this class of columns.

Types of Continuous Columns

Continuous columns can be further classified according to

The nature of the feed that they are processing

- Binary column - feed contains only two components

- Multi-component column - feed contains more than two components

The number of product streams they have

- Multi-product column - column has more than two product streams

Where the extra feed exits when it is used to help with the separation,

- Extractive distillation - where the extra feed appears in the bottom product stream

- Azeotropic distillation - where the extra feed appears at the top product stream

The type of column internals

- Tray column - where trays of various designs are used to hold up the liquid to provide better contact between vapor and liquid, hence better separation

- Packed column - where instead of trays, 'packings' are used to enhance contact between vapor and liquid

MAIN COMPONENTS OF DISTILLATION COLUMNS

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

- A vertical shell where the separation of liquid components is carried out

- Column internals such as trays/plates and/or packings which are used to enhance component separations

- A reboiler to provide the necessary vaporization for the distillation process

- A condenser to cool and condense the vapor leaving the top of the column

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

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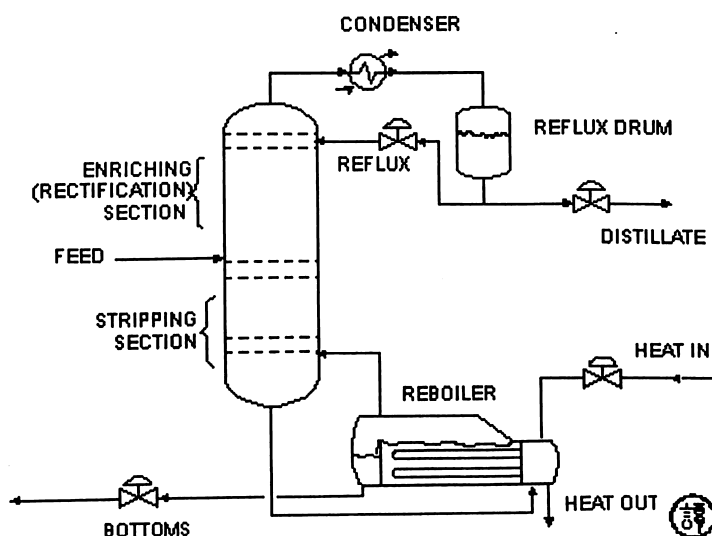
BASIC OPERATION AND TERMINOLOGY

The liquid mixture that is to be processed is known as the feed and this is introduced usually somewhere near the middle of the column to a tray known as the feed tray. The feed tray divides the column into a top (enriching or rectification) section and a bottom (stripping) section. The feed flows down the column where it is collected at the bottom in the reboiler. Heat is supplied to the reboiler to generate vapor. The source of heat input can be any suitable fluid, although in most chemical plants this is normally steam. In refineries, the heating source may be the output streams of other columns. The vapor raised in the reboiler is re-introduced into the unit at the bottom of the column. The liquid removed from the reboiler is known as the bottoms product or simply, bottoms. The vapor moves up the column, and as it exits the top of the unit, it is cooled by a condenser.
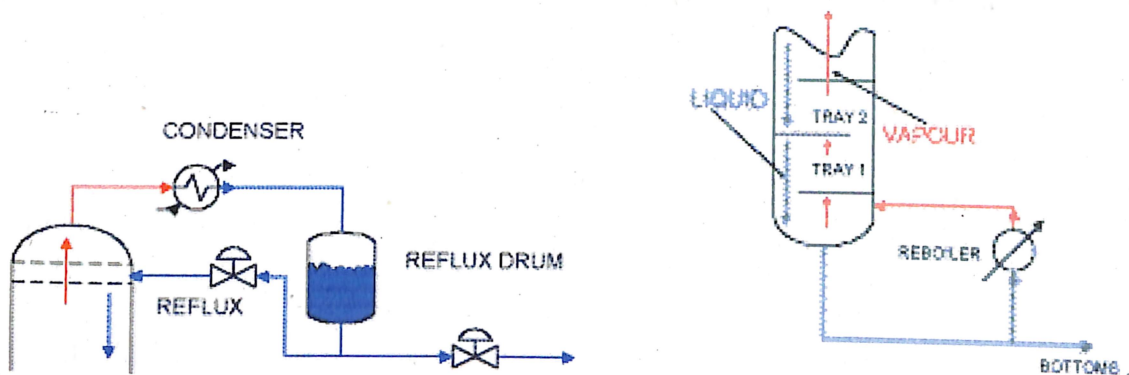
The condensed liquid is stored in a holding vessel known as the reflux drum. Some of this liquid is recycled back to the top of the column and this is called the reflux. The condensed liquid that is removed from the system is known as the distillate or top product. Thus, there are internal flows of vapor and liquid within the column as well as external flows of feeds and product streams, into and out of the column

CHAPTER 2

MULTI – COMPONENT COLUMN MODELING

INTRODUCTION TO MATHEMATICAL MODELING

Mathematical modelling is an important component of all engineering sciences. Modelling involves representation of a process or a system in terms of equations. which best describe its physical nature and/or its working. In practice modelling, is very much an art requiring experience and practice, in addition to a thorough understanding of the physical principles involved.

Modeling of Chemical Engineering Systems can be transport phenomena based, population balance type or empirical. The transport phenomena approach encompasses three basics: mass, energy, and momentum balances applied in their time-varying form. Such a model is termed as an unsteady state model or dynamic model. A steady state model performs the balances over a system, when the properties do not change with time. A perfect steady state is difficult to achieve, but steady state is assumed to prevail if the system behavior does not change significantly with time.

The most important result of developing a mathematical model of a Chemical Engineering system is the understanding and insight gained into the functioning of the system. Models are useful in all phases of Chemical Engineering, from research and development to plant operations, and even in management decision making. In research and development, models can be used to explore the effect of different operating conditions for optimisation and control studies and aid in scale-up studies. In the design phase, models can be used to: explore the sizing and arrangement of processing equipment for dynamic performance; study the interactions of various parts of the process in a recycle system; evaluate alternative process and control structures and strategies; simulate start-up, shutdown, and emergency situations and procedures. In actual plant operation, models help in studying the effects of and the requirements for expansion projects, de-bottlenecking, and optimising plant operations.

The bases for mathematical models are the fundamental physical and chemical laws, such as the law of conservation of mass, energy, and momentum. Models are based upon carefully chosen assumptions. Assumptions are necessary, as an extremely rigorous model that includes every phenomenon down to microscopic

detail would be so complex that, it would take a long time to develop and might be impractical to solve. Assumptions impose limitations on the model that should always be kept in mind when evaluating its predicted results. The most important part of model development is proving that the model describes the real-world situation. A model needs to be validated with experimental or plant operating data. Most often, the model predicted results do not match well with the measured values. The model then needs to be tuned to the plant performance by suitably adjusting the parameters of the model equations. Such parameters are called tuning parameters. The model development is complete when it has been tuned to match the measured variables.

In the present study, the modeling of an atmospheric crude distillation column was undertaken.

ATMOSPHERIC CRUDE DISTILLATION PROCESS

The impact of energy demand for industrialization, development and modern living is widely perceived to be the cause for future wars or strife between the nations of the present day world. In spite of the emergence of studies in non-conventional energy resources, research in the conventional source of energy, the fossil fuel, continues to progress due to its abundance and its significance in the history of industrial development.

Crude oil or petroleum is the most important source of energy and many other consumer products. Its importance can be gauged from the fact that any change in crude prices can alter the world economic order overnight!

Crude oil is a complex mixture of several hundreds of hydrocarbon compounds ranging from simple ethane to very large molecules containing 200 or more carbon atoms. Other than the pure hydrocarbons, the crude contains inorganic impurities in the form of organic compound of sulphur, nitrogen and oxygen. Traces of organo-metallic compounds of iron, nickel, copper, vanadium, arsenic, etc. are also present. Crude oil boils over a wide range of 25 -- 900 °C. Crude oil being a complex mixture needs to be refined into several products, which are tailored to certain specifications depending upon the end use. The principal products of petroleum refining are:

a) Low boiling products: methane, ethane, propane, butane & iso-butane, LPG.

b) Naphtha: light naphtha, heavy naphtha, gasoline or petrol, aviation gasoline.

c) Light distillates: Kerosene, Jet fuels, Aviation Turbine Fuel (ATF).

d) Heavy distillates: Light Gas Oil (LGO), Heavy Gas Oil (HGO), Diesel. e) Vacuum Gas Oils.

f) Lubricating oils & waxes.

g) Residues: fuel oils, coke, asphalt, carbon black etc.

The first process encountered in the course of refining of petroleum in refinery is the *Atmospheric Crude Distillation*. The *Crude Distillation Unit* (CDU) is the core of any petroleum refinery. The crude is fractionated in this unit to yield several distillation products such as Un-stabilized Naphtha or Straight Run Naphtha (SRN), Heavy Naphtha

(HN) or Special Cut Naphtha (SCN), Superior Kerosene (SK) or Aviation Turbine (ATF), Light Gas Oil (LGO), Heavy Gas Oil (HGO) and Reduced Crude Oil (RCO) or Long Residue (LR).

The CDU differs from the conventional distillation column due to the presence of pump-arounds and side-strippers interlinked to the main column. The CDU also lacks a conventional reboiler at the bottom of the main column. The feedstock or the crude oil is desalted and heated to its maximum allowable temperature in a furnace before entering the main column at the flash zone. The flash zone is the area in the CDU where the vaporized feed is allowed to separate from the un-vaporized liquid feed. The vapors rise up through the column and condense on the trays, upon contact with the cold reflux streams coming down. Inter-phase mass transfer takes place primarily on the column trays.

Super heated steam enters the main column from the bottom. Steam serves to strip the liquid teed of its low boiling components iii the stripping section. The bottom liquid is withdrawn from the main column as Long Residue. The main purpose of the steam is to reduce the partial pressure of the hydrocarbons in the vapour phase whereby reducing the temperature required for a given amount of vaporisation.

The overhead vapors from the top tray of the column are cooled in a series of heat exchangers where they are partially condensed. The cooled stream enters the reflux drum, where the non-condensable gases are separated and sent to flare. Water is separated out by virtue of its density and immiscibility with the organic product. Water is drained off from the reflux drum. A part of the liquid is returned to the top tray as reflux and tile rest is withdrawn as distillate product.

There are a number of side-draws in the tower from which the various products like naphtha, kerosene, gas oil etc. are withdrawn. The products are separated according to their boiling ranges. The side-draw products contain some amount of low boiling materials, which are stripped off by superheated steam in the side-strippers. The side-strippers arc generally plate columns into which steam is injected below the bottom tray and the stripped vapors enriched with low boiling materials are returned from the top of the sidestripper to the main column at a location above the withdrawal tray. The desired product stream, free from the low

boiling materials, is drawn from the bottom of the side-stripper.

Pump-arounds are special to the CDU and serve to remove heat from the main column at intermediate points in the rectifying section. The pump-arounds contribute to heat recovery from the CDU at higher temperatures, apart from the top condenser. Pump-arounds ensure more uniform liquid and vapor traffic in the column. The hot liquid is withdrawn from the column and returned to a tray above the with-drawl tray after heat exchange with some cold stream in a heat exchanger.

COLUMN CONFIGURATION

In the present study, the modeling of a crude distillation unit of an operating refinery was considered. The configuration of the *Crude Distillation Unit* (CDU) that is sometimes also referred to as *Heavy Crude Processing Unit (HCU)* is as follows. A schematic diagram of the CDU is shown in Figure 1. 1.

The crude oil from the storage tanks is desalted in a desalter to remove watersoluble salts. It is then heated in a series of exchangers and then fed to a pre-flash drum, which operates at around 4 kg/cm^2 gage pressure and 160°C temperature. The vapors from the pre-flash drum are directly fed to the CDU into the flash zone while the liquid is heated to about 370°C in a series of exchangers and a furnace before it enters the CDU at the flash zone.

The crude distillation unit is a valve tray column with 48 valve trays and 3 chimney trays. Feed is introduced on the 44`h tray (numbering is from the top of the column, the condenser being the first stage). The column is 54 m high. The diameter of the bottom portion of the column (up to tray no. 44) is 2.8m and the top portion is of 4.75m. The flash zone is of 5 meters length. The locations of chimney trays are as first chimney tray falls between trays 5 and 6. The second tray is between trays 14 and i3 and the last one is above 38it' tray. The chimney trays are for vapor distribution only and are not equilibrium stages. The column operates at about 2.5 kg/cm^2 gauge pressure. Superheated steam at 18 kg/cm^2 and 330°C is used for stripping.

The column separates the crude oil into the following six products:

a) Un-stabilized Naphtha (UN) as the top product,

b) Special Cut Naphtha (SCN) as the first draw,

c) Kerosene (SK)/Aviation Turbine Fuel (ATF) as the second draw,

d) Light Gas Oil (LGO) as the third draw,

e) Heavy Gas Oil (HGO) as the fourth draw

f) Long residue (LR) as the bottom draw.

The Un-stabilized Naphtha is obtained as the top distillate from the condenser. The first four draws are taken as the bottom products of the four side-strippers to the main column. The LR is obtained as the bottom product of the column. There are also four pump-arounds (PA) or circulating refluxes (CR).

Side Strippers: HN side stripper is a single pass valve tray column with six trays. The column diameter is 1.2m. Trays are spaced with a distance of 145mm between them. SK side stripper is a two-pass valve tray column with six numbers of trays. Column diameter is 1.8m. LGO side stripper is also a two-pass valve tray column with six numbers of trays, diameter being 1.8m. HGO side stripper has four numbers of valve trays. It is a two-pass column. The diameter of the column is 1.8m and the trays are spaced at a distance of 600mm. Feed to all the stripper columns enters at the top, and the product is drawn at the bottom. Superheated steam (18 kg/cm^2 and 330°C) is injected to the bottom of all the columns to strip off the lighters.

Condenser: The vapors coming out from the top of the column are first cooled in fan cooled finned heat exchangers and then in a water-cooled heat exchanger. The condensed vapors are then sent to a reflux drum where the non-condensable gases and condensed steam are separated out. Water being heavier than the hydrocarbon settles at the bottom of the reflux drum and thus drained off. A part of the condensed liquid hydrocarbon is put back into the main column as reflux while the rest of the liquid, called the Un-stabilized Naphtha (UN) is sent as feed to the Stabilizer where it is further separated into LPG and Stabilized Bottoms. The top tray temperature of the CDU is controlled by manipulating the reflux flow rate. The amount of non-condensable gases in the reflux drum is very less. These non-condensable gases, if any, are burned off in the flare.

MODEL DEVELOPMENT

In the present study, a rigorous model has been developed for a multi - component distillation column of an operating refinery based on the C+3 model equations (C is the number of the pseudo-components in the feed). The conventional tray-by-tray equations are employed for each stage/tray. The model formulation consists of C+3 equations in C+3 independent variables on N trays.

The *C+3 independent variables* for i^{th} equilibrium stage are:

a) Component liquid mole fractions, x_{ij},

b) Total liquid flow rate leaving stage i and reaching stage $i+1$, L_i;

c) Total vapor flow rate leaving stage i and reaching stage $i-1$, V_i and

d) Temperature T_i

The *C+3 model equations* on each equilibrium stage are:

a) Component material balance equations, C in number;

b) Summation equations, two in number and

c) Enthalpy balance equation, one in number.

The *assumptions* made in the development of the model equations are:

a) Liquid on each tray is perfectly mixed and incompressible.

b) Tray vapor holdups are negligible.

c) Dynamics of the condenser have been neglected.

d) Vapor and liquid leaving each stage are in thermal and in phase equilibrium.

e) The partial pressure of water in the condenser has been neglected. The water phase has been considered immiscible with hydrocarbon phase.

f) In the absence of complete operating information about the pre-flash drum, the modeling of the pre-flash drum has not been undertaken. The total feed is assumed to enter the column at the furnace outlet temperature. This may not be a valid assumption.

MODEL EQUATIONS

The model equations for the ith equilibrium stage are listed below. A schematic diagram of an equilibrium stage with all possible input and output streams is shown in the figure below.
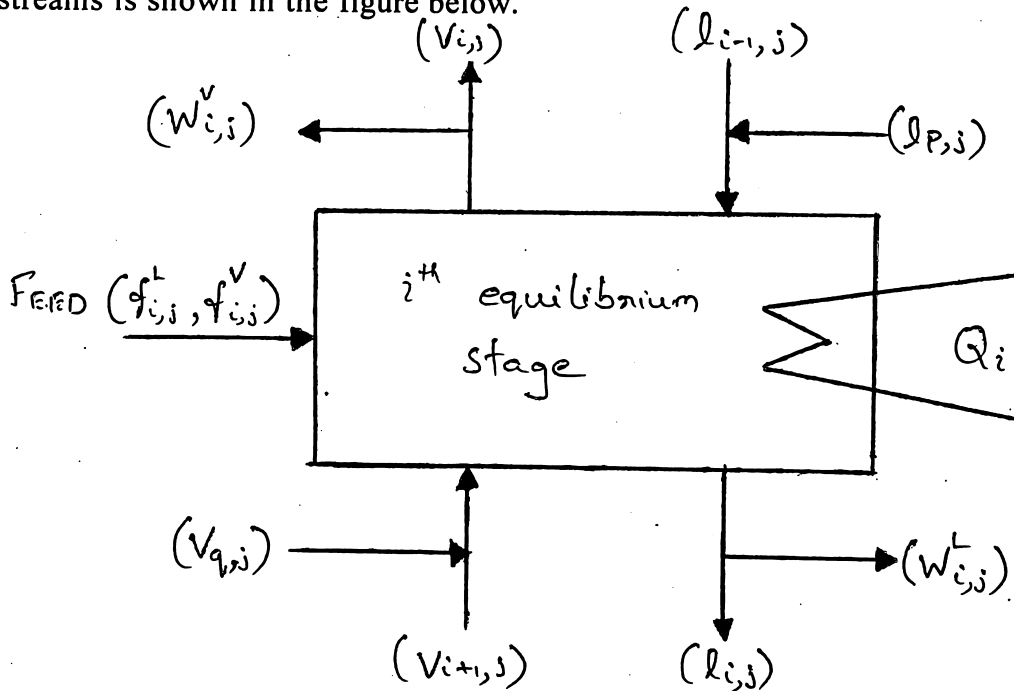
Figure 2.1: A schematic diagram of an equilibrium stage.

1) The *component material balance* equations are:

for i = 1 (condenser),

$$l_{1,j} + d^V_j + d^L_j - v_{2,j} = 0 \; (= M_{1,j}); j = 1,2,\ldots, C \; [Partial \; condenser] \qquad (2.1)$$

$$l_{i,j} + d^L_j - v_{2,j} = 0 \; (= MI_j); j = 1, 2,\ldots, C \quad [Total \; condenser] \qquad (2.2)$$

for i = 2,3... N-1,

$$(l_{i-1,j} + l_{p,j}) + (v_{i+1,j} + v_{q,j}) - (l_{i,j} + w^L_{i,j}) - (v_{i,j} + w^V_{i,j})$$
$$+ f^L_{i,j} + f^V_{i,j} = 0 \; (= M_{i,j}); \qquad\qquad j = 1,2,\ldots, C \qquad (2.3)$$

The liquid feed is assumed to enter from above the tray whereas vapor feed enters from below.

for i = N,

$$v_{N,j} + b_j - l_{N-1,j} = 0 \; (= M_{N,j}); \qquad\qquad j = 1,2,\ldots, C \qquad (2.4)$$

2) The *liquid summation* equation is:

$$L_i - \sum l_{i,i} = 0 \qquad (=S_{Li}); \qquad i = 1, 2, \ldots, N \tag{2.5}$$

3) The *vapor summation* equation is:

$$V_i - \sum v_{i,i} = 0 \qquad (=S_{Vi}); \qquad i = 1, 2, \ldots, N \tag{2.6}$$

In case of total condenser, the summation equation for i=1, is replaced by

$$V_1 - L_1/R_R = 0 \quad (=S_V) \tag{2.7}$$

4) The *enthalpy balance* equations are:

for i=1,

$$\sum l_{1,i} h_{1,j} + \sum d^V_j H^D_j + \sum d^L_j h^D_j - \sum v_{2j} H_{2j} + Q_C = 0 \ (= H_1) \tag{2.8}$$

   [Partial condenser]

$$\sum l_{1,i} h_{1,j} + \sum d^L_j h^D_j + \sum v_{2j} H_{2j} - \sum v_{2j} H_{2j} + Q_C = 0 \ (= H_1) \tag{2.9}$$

   [Total condenser]

for i = 2,3,\ldots\ldots\ldots.N-1

$$\sum l_{i-1,j} h_{i-1,j} + \sum l_{pj} h_{pj} + \sum v_{i+1j} H_{i+1j} - \sum v_{qj} H_{qj}$$

$$- \sum (l_{ij} + w^L_{i,j}) h_{i,j} - \sum (v_{ij} + w^v_{i,j}) H_{ij} + \sum f^L_{ij} h^F_{ij} + \sum f^V_{ij} H^F_{ij} \pm Q_i = 0 \ (= H_i) \tag{2.10}$$

for i=N

$$\sum V_{N,j} H_{N,j} + \sum b_j h^B_j - \sum l_{N-1,j} h_{N-1,j} - Q_N = 0 \ (= H_N) \tag{2.11}$$

5) The *equilibrium relation is:*

$$y_{i,j} = k_{i,j} x_{ij} \tag{2.12}$$

In the above equations following relations hold,

$$l_{i,j} = L_i x_{i,j} \qquad \& \qquad v_{i,j} = V_i K_{i,j} x_{i,j} \tag{2.13}$$

$$w^L_{i,j} = W^L_i x_{i,j} \qquad \& \qquad w^V_{i,j} = W^V_i K_{i,j} x_{i,j} \tag{2.14}$$

$$d^V_j = D^V K_{1,j} x_{i,j} \qquad \& \qquad d^L_j = D^L x_{i,j} \tag{2.15}$$

$$b_j = B^L x_{N,j} \tag{2.16}$$

$$l_{pj} = L_p x_{pj} \tag{2.17}$$

$$v_{qj} = V_q K_{qj} x_{qj} \tag{2.18}$$

In the above equations, l's are component flow rates of liquid streams, v's are component flow rates of vapor streams, w's are component flow rates of side-draws, d's are component flow rates of distillate and b's are component flow rates of bottoms. The liquid enthalpies are denoted by h's and vapor enthalpies by H's. All the flow rates are in lb-moles/hr and the enthalpies are in BTU/(lb-mole).

Equations 2.1 through 2.12 constitute (C+3) relations for each equilibrium stage, thus resulting in a total of N(C+3) non-linear algebraic equations, which are solved simultaneously. Thermodynamic equations are additionally required for the computations of the K-values and the enthalpies at different temperatures and pressures. An initial guess value of all the independent variables used is necessary for the solution of these equations. Since the guess values are not expected to satisfy the equations, discrepancies or error terms are calculated which diminish as iterations proceed. These discrepancies in material balance $(M_{i,j})$, enthalpy balance (H_i) and summation equations (S_{Li} and S_{Vi}) approach zero at convergence.

Specifications

The quantities to be specified in the model equations are:

1) The number of trays/stages in the main column (rectifying and stripping sections), sidestrippers etc.

2) Locations of the feed tray, all the side-stripper streams (in and out) and all the pumparound streams (in and out).

3) Basic physical properties of pseudo-components like their true boiling point, specific gravity, molecular weight, critical temperature, critical pressure and acentric factor.

4) Flow rate, composition and thermal state of the feed entering the column.

5) Condenser temperature or duty.

6) Reflux flow rate or reflux ratio or distillate flow rate.

7) Reflux temperature.

8) Amount of water reflux.

9) Product flow rates from side-strippers and pump-around reflux flow rates.

10) Pump-around return temperatures or heat duties.

11) Flow rates of stripping steam to the main column and the side-strippers or heat

duties of the side-stripper reboilers. Temperature of steam.

12) Column pressure.

The model can be run with two specifications provided at the top of the column. The reflux flow rate and the condenser temperature are specified. The condenser enthalpy balance discrepancy is replaced by,

$$H_i = \quad T_C - T_i \qquad\qquad (2.19)$$

Where,

T_C is the specified condenser temperature.

T_i is the iteration variable for the condenser.

In the material balance equation for the second stage, the quantity $l_{p,j}$ is assigned the amount of specified reflux.

THERMODYNAMIC PROPERTIES

Thermodynamic properties play a crucial role in modeling. There are no exact thermodynamic relations for crude oil due to its inherent complexities and therefore empirical relations are widely used. The correlations for enthalpies and equilibrium constants in the model equations are expressed in terms of the pseudo-component properties, viz., true boiling point, specific gravity, molecular weight, critical temperature, critical pressure and acentric factor. The empirical relations used in this model have been widely tested and their performance was found to be satisfactory.

Enthalpy of liquid and vapor

Kesler and *Lee modification* of Johnson-Grayson charts was used for estimation of liquid and vapor enthalpies of pseudo-components.

Liquid enthalpy $h_j = \int(C_{PL})_j \, dT$ (2.20)

Vapor enthalpy $H_j = \int(C_{PV})_j \, dT + (\Delta H_V)_j$ (2.21)

where,

$(C_{PL})_j$ = Heat capacity of the jth component in liquid phase (BTU/lb-°F).

$(C_{Py})_j$ = Heat capacity of the jth component in vapor phase (BTU/lb-'F).

$(\Delta H_V)_j$ = Heat of vaporization of jth component (BTU/lb).

The expression *for liquid heat capacity is:*

$(C_{PL})_j = (0.6811 - 0.308(Sg)_j + [0.000815 + 0.000306(Sg)_j]T')$ (2.22)
$$* (0.35 + 0.055K_w)$$

The molar enthalpy of the required liquid stream is calculated by adding the pseudo-component enthalpies according to their mole-fractions. The vapor molar enthalpy is also calculated similarly using the following expression for *vapor heat capacity:*

$(C_{PV})_j = A + BT + CT^2 - C_F(A' + B'T + C'T^2)$ (2.23)

where A, B, C, A', B', C' are constants and $C_F = [(12.8/K_w - 1) * (10/K_w - 1) * 100]^2$

In the above expressions, temperature T is °F, K_w is the Watson Characterization factor and $(S_g)_j$ is the specific gravity of jth pseudo-component.

Heat of vaporization: *Lee* and *Kesler [13]* calculated heat of vaporization analytically based on Pitzer's three-parameter corresponding states principle. This method though accurate enough for compounds generally encountered in hydrocarbon processing, the calculation is very rigorous and requires a significant amount of computation time. So, the correlation presented by *Edmister* and *Lee [12]* for calculating heat of vaporization has been used. However, a constant deviation was observed when compared with Lee-Kesler values. Hence, the equation was modified and a constant factor is added to the expression to get a satisfactory result. The expression for heat of vaporization is given below.

$$\Delta(H_V)j = (4.00495 + 5.456344\omega_j) R(T_C)_j (1.8/M_j) + C_1 \qquad (2.24)$$

where,

$\Delta(H_V)j$	=	Heat of vaporization of the jth component (BTU/lb).
R	=	Universal gas constant (= 1.986 BTU/lbmole-°F)
$(T_C)_j$	=	Critical temperature of the jth component in Kelvin.
ω_j	=	Acentric factor of the jth component
M_j	=	Molecular weight of the $j^{`h}$ component.
C_1	=	Constant added for matching the result with that of Lee-

Kesler equations.

Enthalpy of steam

Enthalpy of steam is taken as a polynomial function of temperature. The equation has been regressed using data from steam tables.

$$H_{steam} = 593.044 + 0.46333T + 8.13923X10^{-6}T^2 + 4.89274X10^{-8}T^3 \qquad (2.25)$$

where,

Hsteam	=	Enthalpy of steam in cal/gm.
T	=	Temperature in 'C.

Vapor Liquid Equilibrium

The equilibrium constants (K-values) of lighter paraffins (C_5 and lighters) are calculated using Raoult's law with ideal solution assumption.

$$[K_i]_{Raoult.} = P^s_j / P \qquad\qquad (2.26)$$

where,

K_j $\quad=\quad$ Equilibrium constant of the phase distribution co-efficient of the jth component.

$P_j{}^s$ $\quad=\quad$ Vapor pressure of the jth component in atmospheres.

P $\quad=\quad$ System pressure in atmospheres.

The vapor pressure is calculated from Antoine's equations with modified co-efficients.

$$ln(P_j^s) = A + B/(C+T) \qquad\qquad (2.27)$$

Where,

A $\qquad\qquad=\qquad$ 6.8736

B $\qquad\qquad=\qquad$ 967.27 + 2.89$(T_B)_j$

C $\qquad\qquad=\qquad$ 244.53 - 0.2977$(T_B)_j$

T $\qquad\qquad=\qquad$ System temperature in Kelvin.

$(T_B)_j$ $\qquad=\qquad$ Normal boiling point for the jth component in Kelvin.

Steam Condensation

In the condenser, the water phase has been assumed immiscible with the hydrocarbon phase and its partial pressure has been neglected. The measured temperature on the top tray of the CDU is about 100-110 °C and the pressure at the top of the column is about 3.5 kg/cm^2 absolute. The saturation temperature of water at this pressure is 135 °C. Therefore the operating temperatures of the top few trays are lower than the saturation temperature of water and hence the presence of a third phase, water in these trays was expected. Condensation of steam, though in small amounts, in these trays would affect the enthalpy balance due to its high latent heat of vaporization. A careful study of the top tray thermodynamics revealed that condensation of steam doesn't occur on these trays at the prevailing operating conditions of the column.

Water and petroleum fractions are assumed to be immiscible with each other. Although no two liquids are totally immiscible, this condition is closely

approached by several systems and these can be idealized as completely immiscible.

Applying low pressure VLE relations to the three phase equilibrium point B, it can be noticed that at a specified system pressure P^* if two immiscible liquid phases are in equilibrium with the vapor phase, the three phase equilibrium temperature T^* is less than the saturation temperature of either liquid at the specified pressure. The three phase equilibrium temperature T^* at system pressure P^* satisfies the following relation:

$$P^* = P_1^S + P_2^S \qquad (2.28)$$

The vapor composition at the three-phase equilibrium point B is given by:

$$y^B_1 = P_1^S / (P_1^S + P_2^S) \qquad (2.29)$$

where, P_1^S and P_2^S are the saturation pressures of components 1 and 2 at temperature T^*.

SOLUTION PROCEDURE

Though a solution of the model is not in the purview of the project, a theoretical solution procedure is covered here so as to get an overall idea.

The steady state model for the CDU consists of $N(C+3)$ non-linear algebraic equations. The number of equations is very large due to the large number of stages in the CDU. These equations are solved simultaneously by a modified Newton-Raphson technique, until the values of the residual functions are below the specified tolerance. The equations expressed in terms of vectors are as follows.

$X = [X_1, X_2, X_3, \ldots\ldots X_N]^T$

$F = [F_1, F_2, F_3, \ldots\ldots\ldots F_N]^T$

X, is the vector of independent variables and F; is the vector of the discrepancies on the stage.

The Newton-Raphson iterative formula is given by,

$$X^{k+1} = X^k + \beta^k (\Delta X^k)$$ (2.30)

where,

β is the non-negative move suppression factor with $0<\beta<1$, and k is the iteration number.

ΔX^k is the change in the independent variables set for the kth iteration, obtained from Taylor's expansion, neglecting the higher order derivatives and is added in proper proportion to get the new independent variable set for the $(k+1)^{th}$ iteration.

The change AV can be calculated from the following relation

$$J^k \Delta X^k = -F^k$$ (2.31)

where, J^k is the Jacobian matrix of the first partial derivatives given by,

For the stages without side-streams, the above Jacobian matrix contains the non-zero terms corresponding to the ith, $(i-1)^{th}$ and $(i+1)^{th}$ stages only, thus giving rise to a tri-diagonal band. In the case of stages with side-streams, like side-strippers and/or pump around draw/return trays, non-zero terms appear at off tri-diagonal positions. In the present formulation, each non-zero term of the above Jacobian matrix is a sub matrix of $[(C+3) \times (C+3)]$ dimension. The elements of the sub matrix in the ith row and jth column are the partial derivatives of functions (material and energy balance discrepancy functions) on the ith stage with respect to the independent variables of the jth stage. All these partial derivatives can be calculated numerically or analytically.

In the present study, analytical derivatives have been used to compute the partial derivatives. The main disadvantage of using numerical derivatives is that it takes more computation time compared to the derivatives calculated analytically. The magnitude of the perturbation also affects the convergence either in the accuracy of the results (in turn depends on the sensitivity of the variables) or in time, or in both.

CHAPTER 3

SIMULATION

OVERVIEW

There are two types of simulations in process modeling:

1) Flow sheeting
2) Equation oriented

While Matlab and gPROMS come under equation oriented simulations, Aspen is a method of flow sheeting. Aspen is the main context in the project undertaken. There are various modules in Aspen such as Aspen Hysis, Aspen Plus, Aspen DMC Plus, Aspen Pims and Aspen Infoplus.

The main advantages of Aspen Hysis are:

- Event Driven Operation
- Modular Operations
- Multi-flow sheet Architecture
- Object Oriented Design

The primary interface elements in Aspen Hysis are:

Interface Element	Description
PFD	Graphical Environment
Workbook	Collection of Tabs
Property View	Information about Specific Object
Summary View	Displays Currently Installed Streams
Simulation Navigation	Simulation Case

COLUMN SIMULATION

A CASE STUDY

This case summarizes a typical short multi-component distillation. Here the problem is to separate component 4 from component 5 while keeping component 5 losses into the overhead at less than 5 weight % of the total overhead or to recover the bottoms better than 90% (weight) of the component 5 entering in the feed.

The feed composition is:

Component	Mols	Pounds	Boil Point, °F
1	0.623	53.68	155.7
2	7.234	130.36	313.0
3	80.223	7423.03	244.2
4	1.717	127.20	332.6
5	9.678	1395.28	380.3
6	0.525	85.37	476.6
	----------	------------	
	100.00	9214.91	

Enthalpy: BTU/unit flow 2901.076 31.48

Feed temperature: 90°F, liquid at stage 5 from top, Equimolal overflow not assumed.

Column Pressure: 0.39 (top) to 0.86 (bottom) psia, distributed uniformly to each tray

Reflux Ratio: 0.50 (assumed)

Assumed no. theoretical stages: 8 including condenser and reboiler

Summary of input data to computer:

1. Molecular weights
2. Boiling points
3. "K" value equations for each component as a function of pressure
4. Equations for calculating enthalpy of liquid of each component as a function of temperature

5. Equations for calculating enthalpy of vapor of each component as a function of temperature

6. *Initial* values for stages to start calculations

    a. Linear temperature gradient

    b. Linear pressure gradient

INPUT DATA

The following data has been used as input values for the simulation.

Computer Printout for Multi-component Distillation

NUMBER OF STAGES =   8   (INCLUDING CONDENSER AND REBOILER)
NUMBER OF COMPONENTS = 6

COMPONENTS	MOLECULAR WEIGHT	NORMAL BOILING POINT, DEG. F.
1	86.170	155.70
2	18.020	212.00
3	92.530	244.20
4	74.080	332.60
5	144.17	380.30
6	162.61	476.60

COLUMN PRESSURE =   0.39   TO   0.86 PSIA
REFLUX RATIO =   0.5000

EQUIMOLAL OVERFLOW NOT ASSUMED

FEED STREAMS

STAGE   5   (LIQUID FEED STREAM), TEMP. =   90.00 DEG.F.

COMPONENT	MOLS	LBS.
1	0.623	53.68
2	7.234	130.36
3	80.223	7423.03
4	1.717	127.20
5	9.678	1395.28
6	0.525	85.37
TOTAL	100.000	9214.91
ENTHALPY, BTU/ UNIT FLOW	2901.076	31.48

SUM OF FEEDS = 100.000 MOLS

PRODUCT STREAMS

OVERHEAD RATE   =   89.797   MOLS LIQUID
                          0.0   MOLS VAPOR

BOTTOMS RATE   =   10.203 MOLS LIQUID

SUM OF PRODUCTS = 100.000 MOLS

INITIAL VALUES FOR STAGE VARIABLES (LINEAR TEMP. GRADIENT, LINEAR PRESSURE GRADIENT, EQUIMOLAL OVERFLOW, SPECIFIED HEAT LOSSES NOT INCLUDING OVERHEAD CONDENSER AND BOTTOMS REBOILER)

STAGE	TEMP.DEG.F	PRESS.PSIA	L (MOLS)	V (MOLS)	Q (BTU)
1	85.00	0.39	144.898	0.0	0.0
2	102.86	0.46	144.898	134.695	0.0
3	120.71	0.52	144.898	134.695	0.0
4	138.57	0.59	144.898	134.695	0.0
5	156.43	0.66	144.898	134.695	0.0
6	174.29	0.73	144.898	134.695	0.0
7	192.14	0.79	144.898	134.695	0.0
8	210.00	0.86	10.203	134.695	0.0

STAGE NO.   1.................... OVERHEAD CONDENSER

TEMPERATURE =   81.75 DEG.F
PRESSURE =   0.39 PSIA

STAGE NO.   2

TEMPERATURE =   95.98 DEG.F
PRESSURE =   0.46 PSIA

STAGE NO. 3

                TEMPERATURE =   115.04 DEG.F
                PRESSURE =   0.52 PSIA

STAGE NO. 4

                TEMPERATURE =   131.91 DEG.F
                PRESSURE =   0.59 PSIA

STAGE NO. 5

                TEMPERATURE =   144.67 DEG.F
                PRESSURE =   0.66 PSIA

STAGE NO. 6

                TEMPERATURE =   188.49 DEG.F
                PRESSURE =   0.73 PSIA

STAGE NO. 7

                TEMPERATURE =   213.25.75 DEG.F
                PRESSURE =   0.79 PSIA

STAGE NO. 8   (REBOILER ------ LIQUID STREAM IS BOTTOMS PRODUCT)

                TEMPERATURE =   224.68 DEG.F
                PRESSURE =   0.86 PSIA

          REBOILER HEAT DUTY =   2573009.0 BTU
          CONDENSER HEAT DUTY =   2499393.0 BTU

OVERALL COMPONENT BALANCES (MOLS)   ----- BEFORE FINAL FORCING -----

	IN	OUT	IN/OUT
1	0.62300	0.62300	1.00000000
2	7.23400	7.23400	1.00000000
3	80.22301	80.22293	1.00000000
4	1.71700	1.71700	1.00000000
5	9.67800	9.67804	0.99999583
6	0.52500	0.52500	0.99999529
	99.99998	99.99995	1.00000000

RESULTS AND DISCUSSIONS

The column has been modeled using Peng-Robinson and Redlich-Kwong-Soave (SRK) correlation.

COLUMN ENVIRONMENT
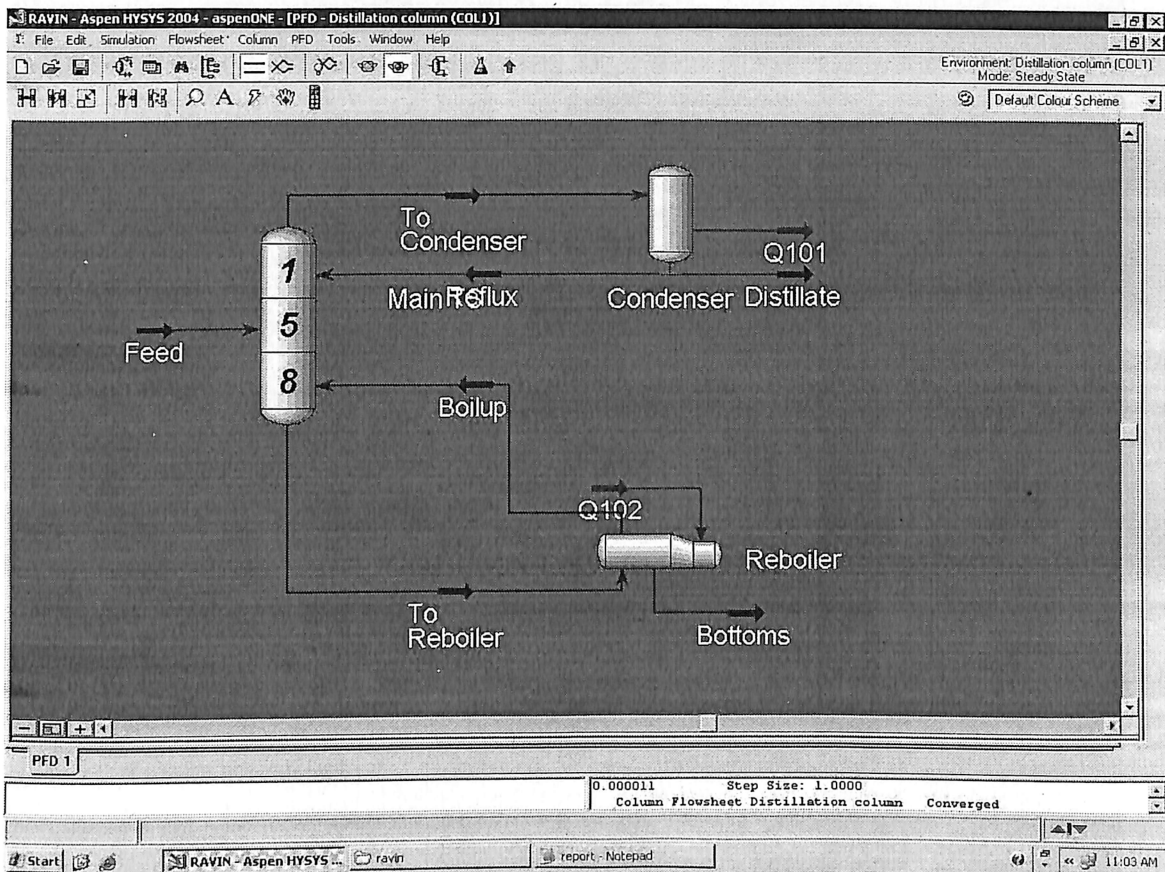
- Stage 5 is the feed stage where the liquid feed stream enters at 90°F
- Stage 1 and stage 8 are the product streams
- Stage 1 is the overhead product stream where the vapor stream is connected the overhead condenser.
- Stage 8 is the bottoms product stream where the liquid stream is connected to the reboiler.
- Components 1, 2, 3 and 4 are light while components 5 & 6 are heavy.

PARENT ENVIRONMENT
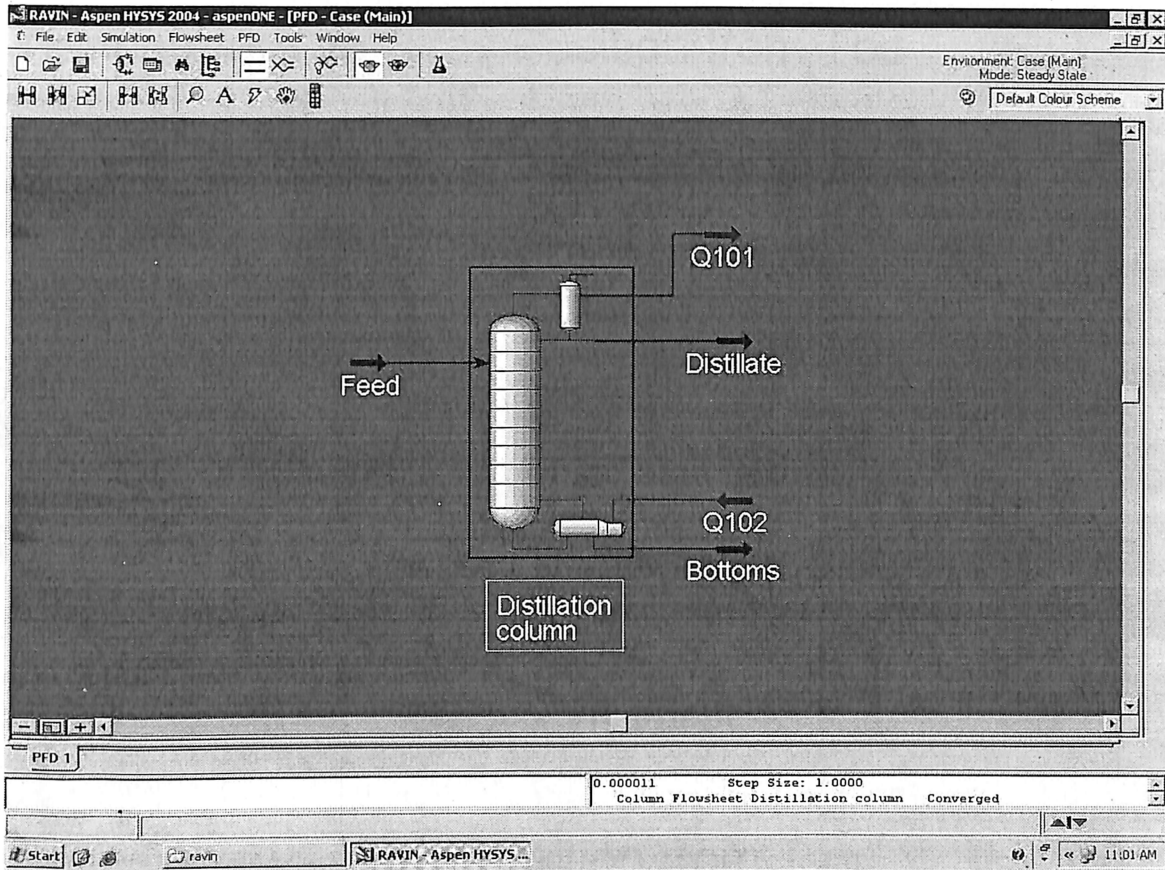
PLOTS

Temperature vs. Tray Position from Top
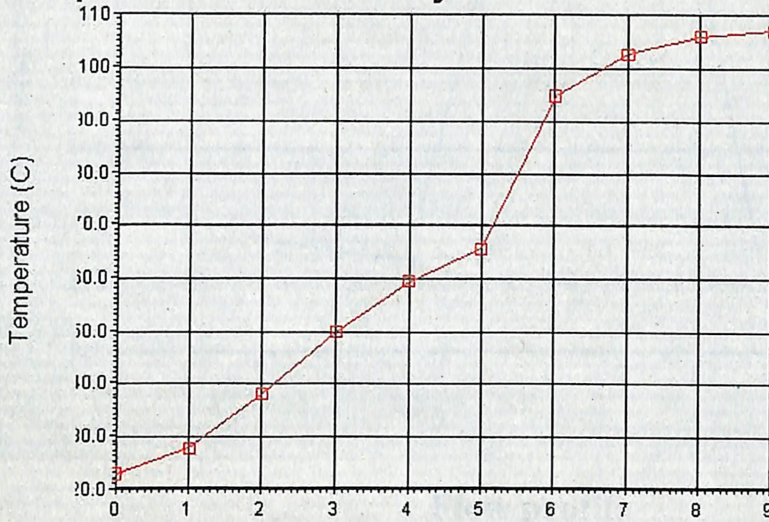
Temperature profile

Pressure vs. Tray Position from Top
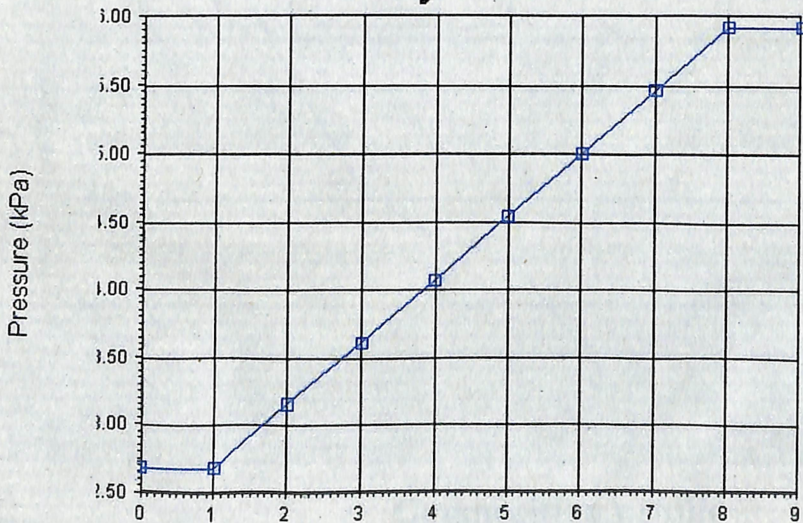
Pressure profile

Flow vs. Tray Position from Top
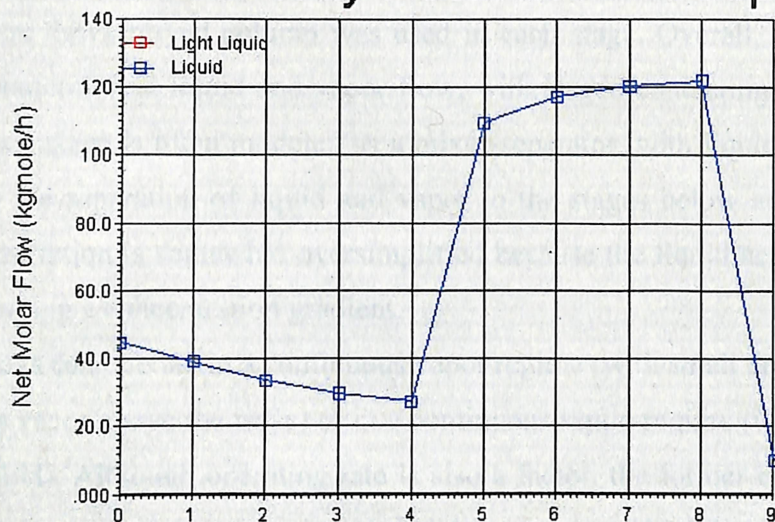
Flow profile

Composition vs. Tray Position from Top
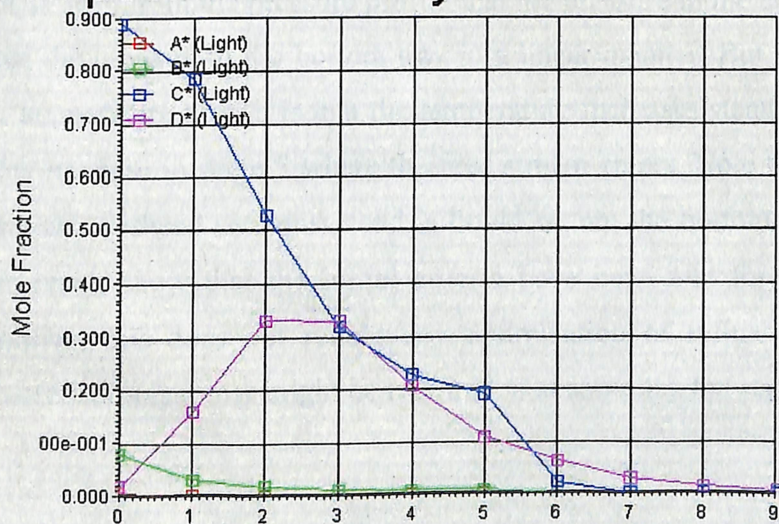
Composition profile

Here Sieve trayed column was used in each stage. Overall, trayed columns operate via countercurrent liquid and vapor flow, with staged contacting for heat and mass transfer. Each stage is often modeled as a mixer-separator, with liquid-vapor contacting followed by the separation of liquid and vapor to the stages below and above respectively. This description is somewhat oversimplified because the liquid actually flows across the tray, creating a concentration gradient.

Trays can operate in a continuous vapor regime (with small droplets of liquid dispersed in the vapor above the trays) or in a continuous liquid regime (with bubbles dispersed in the liquid). Although operating rate is also a factor, the former condition is characteristic of vacuum columns and the latter of high pressure and high liquid flow rate columns. "Sieve trays are less expensive than bubble-cap or valve trays because they are the simplest to make".

The results of the simulations are as summarized by copies of the workbook printouts[1]. It can be seen from the pressure profile that the pressure in the column is steadily increasing from the top tray to the bottom tray in a linear manner. But what can be observed from the temperature profile is that the temperature increases steadily till stage 5 but there is a steep increase in stage 5 where the feed stream enters. Note that stage *one* is the product from an overhead condenser and is liquid, as are the bottoms or reboiler outlet product. The result show that the initial criteria have been met for recovery of component 5; however, this does not reflect any optimization of reflux or final number of stages (theoretical trays) that might be required to accomplish the separation in a final design.

NOMENCLATURE

C   = number of components.

b_j = flow rate of jth component in the bottom product.

B^L = total flow rate of the bottom product (liquid).

d^L_j = flow rate of jth component in the liquid distillate.

d^V_j = flow rate of jth component in the vapor distillate.

D^L = total flow rate of the liquid distillate.

D^V = total flow rate of the vapor distillate.

$f^L_{i,j}$ = flow rate of jth component in the liquid feed on the ith stage.

$f^V_{i,j}$ = flow rate of jth component in the vapor feed on the ith stage.

F_{obj} =objective function.

h^B_j = enthalpy of jth component in the bottom product.

h^D_j = enthalpy of jth component in the liquid distillate.

$h^F_{i,j}$ = enthalpy of jth component in the liquid feed on the ith stage.

$h_{i,j}$ = enthalpy of jth component in the liquid leaving the ith stage.

$h_{p,j}$ = enthalpy of jth component in the liquid from the pth stage reaching the ith stage.

H^D_j =enthalpy of jth component in the vapor distillate.

$H^F_{i,j}$ = enthalpy of jth component in the vapor feed on the ith stage.

$H_{i,j}$ = enthalpy of jth component in the vapor leaving the ith stage.

$H_{q,j}$ = enthalpy of jth component in the vapor from the qth stage reaching the ith stage.

H_i = discrepancy in enthalpy balance on the ith stage.

K_w = Watson's characterization factor.

$K_{i,j}$ = equilibrium constant of the jth component on the ith plate.

$l_{i,j}$ = liquid flow rate of jth component leaving the ith stage and reaching the $(i+1)^{th}$ stage.

$l_{p,j}$ = liquid flow rate of jth component from the pth stage reaching the ith.

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APPENDIX

Distillation: Distillation column @Main

CONNECTIONS

Inlet Stream

STREAM NAME	Stage	FROM UNIT OPERATION
Q102	Reboiler	
Feed	5 Main TS	

Outlet Stream

STREAM NAME	Stage	TO UNIT OPERATION
Q101	Condenser	
Distillate	Condenser	
Bottoms	Reboiler	

MONITOR

Specifications Summary

	Specified Value	Current Value	Wt. Error	Wt. Tol.	Abs. Tol.	Active	Estimate	Used
Reflux Ratio	0.5000 *	0.5000	3.295e-007	1.000e-002 *	1.000e-002 *	On	On	On
Distillate Rate	89.80 kgmole/h *	89.80 kgmole/h	3.276e-007	1.000e-002 *	1.000 kgmole/h *	On	On	On
Btms Prod Rate	10.20 kgmole/h *	10.20 kgmole/h	-2.883e-006	1.000e-002 *	1.000 kgmole/h *	Off	On	Off
Comp Recovery	0.9000 *	0.9684	3.473e-002	1.000e-002 *	1.000e-003 *	Off	On	Off

SPECS

Column Specification Parameters

Reflux Ratio

Fixed / Ranged:	Fixed	Primary / Alternate:	Primary	Lower Bound:	—	Upper Bound:	—
Stage:	Condenser	Flow Basis:	Molar	Liquid Specification:	—		

Distillate Rate

Fixed / Ranged:	Fixed	Primary / Alternate:	Primary	Lower Bound:	—	Upper Bound:	—
Stream:	Distillate	Flow Basis:	Molar				

Btms Prod Rate

Fixed / Ranged:	Fixed	Primary / Alternate:	Primary	Lower Bound:	—	Upper Bound:	—
Stream:	Bottoms	Flow Basis:	Molar				

Comp Recovery

Fixed / Ranged:	Fixed	Primary / Alternate:	Primary	Lower Bound:	—	Upper Bound:	—
Draw:	Distillate	Flow Basis:	Molar				
Components:	D*						

SUBCOOLING

	Condenser	
Degrees of Subcooling		—
Subcool to		—

User Variables

PROFILES

General Parameters

Sub-Flow Sheet:	Distillation column (COL1)	Number of Stages:	8 *

Profile Estimates

	Temperature (C)	Net Liquid (kgmole/h)	Net Vapour (kgmole/h)
Condenser	27.64 *	44.90	2.014e-020

Distillation: Distillation column @Main (continued)

Profile Estimates

	Temperature (C)	Net Liquid (kgmole/h)	Net Vapour (kgmole/h)
1__Main TS	35.54 *	39.58	134.7
2__Main TS	38.05	33.91	129.4
3__Main TS	49.89	29.74	123.7
4__Main TS	59.41	27.44	119.5
5__Main TS	65.62	109.6	117.2
6__Main TS	94.87	117.4	99.44
7__Main TS	103.1	120.7	107.2
8__Main TS	106.2	122.1	110.5
Reboiler	107.0 *	10.20	111.9

EFFICIENCIES

Stage Efficiencies

Stages	Overall Efficiency	A*	B*	C*	D*	E*
Condenser	1.000	1.000	1.000	1.000	1.000	1.000
1__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
2__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
3__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
4__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
5__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
6__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
7__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
8__Main TS	1.000	1.000	1.000	1.000	1.000	1.000
Reboiler	1.000	1.000	1.000	1.000	1.000	1.000

Stages	Overall Efficiency	F*				
Condenser	1.000	1.000				
1__Main TS	1.000	1.000				
2__Main TS	1.000	1.000				
3__Main TS	1.000	1.000				
4__Main TS	1.000	1.000				
5__Main TS	1.000	1.000				
6__Main TS	1.000	1.000				
7__Main TS	1.000	1.000				
8__Main TS	1.000	1.000				
Reboiler	1.000	1.000				

SOLVER

Column Solving Algorithm: HYSIM Inside-Out

Solving Options		Acceleration Parameters	
Maximum Iterations:	10000	Accelerate K Value & H Model Parameters:	Off
Equilibrium Error Tolerance:	1.000e-05		
Heat/Spec Error Tolerance:	5.000e-004		
Save Solutions as Initial Estimate:	On		
Super Critical Handling Model:	Simple K		
Trace Level:	Low	**Damping Parameters**	
Init from Ideal K's:	Off	Azeotrope Check:	Off
Initial Estimate Generator Parameters		Fixed Damping Factor:	1
Iterative IEG (Good for Chemicals):	Off		

SIDE STRIPPERS

Distillation: Distillation column @Main (continued)

SIDE RECTIFIERS

PUMP AROUNDS

VAP BYPASSES

RATING

Tray Sections

Tray Section		Main TS			
Tray Diameter	(m)	1.500 *			
Weir Height	(m)	5.000e-002 *			
Weir Length	(m)	1.200 *			
Tray Space	(m)	0.5500 *			
Tray Volume	(m3)	0.9719			
Disable Heat Loss Calculations		No			
Heat Model		None			
Rating Calculations		No			
Tray Hold Up	(m3)	8.836e-002			

Vessels

Vessel		Reboiler	Condenser		
Diameter	(m)	1.193	1.193		
Length	(m)	1.789	1.789		
Volume	(m3)	2.000 *	2.000 *		
Orientation		Horizontal	Horizontal		
Vessel has a Boot		No	No		
Boot Diameter	(m)	---	---		
Boot Length	(m)	---	---		
Hold Up	(m3)	1.000	1.000		

Other Equipment In Column Flowsheet

Pressure Profile

	Pressure (kPa)		Pressure Drop (kPa)
Condenser	2.689 kPa *		0.0000 kPa
1__Main TS	2.689 kPa		0.4629 kPa
2__Main TS	3.152 kPa		0.4629 kPa
3__Main TS	3.615 kPa		0.4629 kPa
4__Main TS	4.078 kPa		0.4629 kPa
5__Main TS	4.541 kPa		0.4629 kPa
6__Main TS	5.004 kPa		0.4629 kPa
7__Main TS	5.467 kPa		0.4629 kPa
8__Main TS	5.929 kPa		---
Reboiler	5.929 kPa *		0.0000 kPa

Pressure Solving Options

Pressure Tolerance	1.000e-004 *	Pressure Drop Tolerance	1.000e-004 *	Damping Factor	1.000 *	Max Press Iterations	100 *

CONDITIONS

Name	Feed @Main	Distillate @Main	Bottoms @Main	Q102 @Main	Q101 @Main
Vapour	0.0000 *	0.0000	0.0000	---	---

Distillation: Distillation column @Main (continued)

CONDITIONS

Temperature	(C)	32.2222 *	23.0820	107.3732	—	—
Pressure	(kPa)	3.8835	2.6890	5.9295	—	—
Molar Flow	(kgmole/h)	100.0000 *	89.7970	10.2030	—	—
Mass Flow	(kg/h)	9214.9175	7738.0915	1476.8260	—	—
Std Ideal Liq Vol Flow	(m3/h)	12.1184	10.2858	1.8326	—	—
Molar Enthalpy	(kJ/kgmole)	-2.080e+005	-1.973e+005	-2.937e+005	—	—
Molar Entropy	(kJ/kgmole-C)	110.7	90.73	278.0	—	—
Heat Flow	(kJ/h)	-2.0801e+07	-1.7720e+07	-2.9967e+06	5.5169e+06	5.4327e+06

PROPERTIES

Name		Feed @Main	Distillate @Main	Bottoms @Main		
Molecular Weight		92.15 *	86.17 *	144.7 *		
Molar Density	(kgmole/m3)	8.207 *	8.770 *	5.071 *		
Mass Density	(kg/m3)	756.3 *	755.7 *	734.0 *		
Act. Volume Flow	(m3/h)	12.18 *	10.24 *	2.012 *		
Mass Enthalpy	(kJ/kg)	-2257 *	-2290 *	-2029 *		
Mass Entropy	(kJ/kg-C)	1.201 *	1.053 *	1.921 *		
Heat Capacity	(kJ/kgmole-C)	196.9 *	183.1 *	333.7 *		
Mass Heat Capacity	(kJ/kg-C)	2.137 *	2.125 *	2.306 *		
Lower Heating Value	(kJ/kgmole)	—	—	—		
Mass Lower Heating Value	(kJ/kg)	—	—	—		
Phase Fraction [Vol. Basis]		—	—	—		
Phase Fraction [Mass Basis]		2.122e-314 *	2.122e-314 *	2.122e-314 *		
Partial Pressure of CO2	(kPa)	0.0000 *	0.0000 *	0.0000 *		
Cost Based on Flow	(Cost/s)	0.0000 *	0.0000 *	0.0000 *		
Act. Gas Flow	(ACT_m3/h)	—	—	—		
Avg. Liq. Density	(kgmole/m3)	8.252 *	8.730 *	5.567 *		
Specific Heat	(kJ/kgmole-C)	196.9 *	183.1 *	333.7 *		
Std. Gas Flow	(STD_m3/h)	2364 *	2123 *	241.2 *		
Std. Ideal Liq. Mass Density	(kg/m3)	760.4 *	752.3 *	805.9 *		
Act. Liq. Flow	(m3/s)	3.384e-003 *	2.844e-003 *	5.589e-004 *		
Z Factor		—	1.245e-004 *	3.696e-004 *		
Watson K		11.77 *	11.80 *	11.71 *		
User Property		—	—	—		
Partial Pressure of H2S	(kPa)	0.0000 *	0.0000 *	0.0000 *		
Cp/(Cp - R)		1.044 *	1.048 *	1.026 *		
Cp/Cv		1.197 *	1.207 *	1.139 *		
Heat of Vap.	(kJ/kgmole)	4.534e+004 *	4.033e+004 *	5.066e+004 *		
Kinematic Viscosity	(cSt)	0.7407 *	0.7323 *	0.6099 *		
Liq. Mass Density (Std. Cond)	(kg/m3)	771.3 *	762.9 *	806.4 *		
Liq. Vol. Flow (Std. Cond)	(m3/h)	11.95 *	10.14 *	1.831 *		
Liquid Fraction		1.000 *	1.000 *	1.000 *		
Molar Volume	(m3/kgmole)	0.1218 *	0.1140 *	0.1972 *		
Mass Heat of Vap.	(kJ/kg)	492.0 *	468.1 *	350.0 *		
Phase Fraction [Molar Basis]		0.0000 *	0.0000 *	0.0000 *		
Surface Tension	(dyne/cm)	22.13 *	22.71 *	18.69 *		
Thermal Conductivity	(W/m-K)	0.1452 *	0.1479 *	0.1268 *		
Viscosity	(cP)	0.5602 *	0.5534 *	0.4477 *		
Cv (Semi-Ideal)	(kJ/kgmole-C)	188.6 *	174.8 *	325.4 *		
Mass Cv (Semi-Ideal)	(kJ/kg-C)	2.047 *	2.029 *	2.248 *		
Cv	(kJ/kgmole-C)	164.6 *	151.7 *	292.9 *		
Mass Cv	(kJ/kg-C)	1.786 *	1.760 *	2.024 *		

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* Specified by user.

Distillation: Distillation column @Main (continued)

PROPERTIES

Name		Feed @Main	Distillate @Main	Bottoms @Main		
Cv (Ent. Method)	(kJ/kgmole-C)	—	—	—		
Mass Cv (Ent. Method)	(kJ/kg-C)	—	—	—		
Cp/Cv (Ent. Method)		—	—	—		
Reid VP at 37.8 C	(kPa)	5.091 *				
True VP at 37.8 C	(kPa)	5.108 *	5.665 *	0.1571 *		
Liq. Vol. Flow - Sum(Std. Cond)	(m3/h)	11.95 *	10.14 *	1.831 *		

SUMMARY

Flow Basis:			Molar	The composition option is selected		

Feed Composition

	Feed					
Flow Rate (kgmole/h)	100.0000					
	—					
A*	0.0062					
B*	0.0723					
C*	0.8022					
D*	0.0172					
E*	0.0968					
F*	0.0053					

Flow Basis:		Molar	The composition option is selected		

Feed Flows

	Feed				
Flow Rate (kgmole/h)	100.0000				
	—				
A* (kgmole/h)	0.6230				
B* (kgmole/h)	7.2340				
C* (kgmole/h)	80.2230				
D* (kgmole/h)	1.7170				
E* (kgmole/h)	9.6780				
F* (kgmole/h)	0.5250				

Products

Flow Basis:		Molar	The composition option is selected		

Product Compositions

	Distillate	Bottoms			
Flow Rate (kgmole/h)	89.7970	10.2030			
	—	—			
A*	0.0069	0.0000			
B*	0.0806	0.0000			
C*	0.8934	0.0000			
D*	0.0185	0.0053			
E*	0.0006	0.9432			
F*	0.0000	0.0515			

Flow Basis:		Molar	The composition option is selected		

Product Flows

	Distillate	Bottoms			
Flow Rate (kgmole/h)	89.7970 *	10.2030 *			
	—	—			
A* (kgmole/h)	0.6230 *	0.0000 *			
B* (kgmole/h)	7.2340 *	0.0000 *			
C* (kgmole/h)	80.2228 *	0.0002 *			
D* (kgmole/h)	1.6627 *	0.0543 *			

HYPROTECH
LIFECYCLE INNOVATION

UNIVERSITY OF PETROLEUM
Calgary, Alberta
CANADA

Case Name:	X:\DESKTOP\RAVIN\RAVIN.HSC
Unit Set:	SI
Date/Time:	Wed Apr 25 11:26:58 2007

Distillation: Distillation column @Main (continued)

SUMMARY

	Distillate	Bottoms			
E* (kgmole/h)	0.0545 *	9.6235 *			
F* (kgmole/h)	0.0000 *	0.5250 *			
Flow Basis:		Molar	The composition option is selected		

Product Recoveries

	Distillate	Bottoms			
Flow Rate (kgmole/h)	89.7970	10.2030			
	—	—			
A* (%)	100.0000	0.0000			
B* (%)	100.0000	0.0000			
C* (%)	99.9998	0.0002			
D* (%)	96.8354	3.1646			
E* (%)	0.5635	99.4365			
F* (%)	0.0000	100.0000			

COLUMN PROFILES

Reflux Ratio:	0.5000	Reboil Ratio:	10.97	The Flows Option is Selected	Flow Basis:	Molar

Column Profiles Flows

	Temperature (C)	Pressure (kPa)	Net Liq (kgmole/h)	Net Vap (kgmole/h)	Net Feed (kgmole/h)	Net Draws (kgmole/h)
Condenser	23.08	2.689	44.90	—	—	89.80
1__Main TS	27.81	2.689	39.58	134.7	—	—
2__Main TS	38.05	3.152	33.91	129.4	—	—
3__Main TS	49.89	3.615	29.74	123.7	—	—
4__Main TS	59.41	4.078	27.44	119.5	—	—
5__Main TS	65.62	4.541	109.6	117.2	100.0	—
6__Main TS	94.87	5.004	117.4	99.44	—	—
7__Main TS	103.1	5.467	120.7	107.2	—	—
8__Main TS	106.2	5.929	122.1	110.5	—	—
Reboiler	107.4	5.929	—	111.9	—	10.20

Column Profiles Energy

	Temperature (C)	Liquid Enthalpy (kJ/kgmole)	Vapour Enthalpy (kJ/kgmole)	Heat Loss (kJ/h)
Condenser	23.08	-1.973e+005	-1.466e+005	—
1__Main TS	27.81	-2.019e+005	-1.570e+005	—
2__Main TS	38.05	-2.082e+005	-1.568e+005	—
3__Main TS	49.89	-2.299e+005	-1.564e+005	—
4__Main TS	59.41	-2.544e+005	-1.600e+005	—
5__Main TS	65.62	-2.694e+005	-1.644e+005	—
6__Main TS	94.87	-2.862e+005	-2.114e+005	—
7__Main TS	103.1	-2.901e+005	-2.341e+005	—
8__Main TS	106.2	-2.915e+005	-2.398e+005	—
Reboiler	107.4	-2.937e+005	-2.420e+005	—

FEEDS / PRODUCTS

Flow Basis:				Molar			
	Stream	Type	Duty (kJ/h)	State	Flows (kgmole/h)	Enthalpy (kJ/kgmol)	Temp (C)
Condenser	Q101	Energy	5.433e+006 *		—	—	—
	Distillate	Draw	—	Liquid	89.80 *	-1.973e+005 *	23.08 *
1__Main TS							
2__Main TS							
3__Main TS							
4__Main TS						100.0	-2.080e+005 *	32.22 *
5__Main TS	Feed	Feed	—	Liquid			

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* Specified by user.

Distillation: Distillation column @Main (continued)

FEEDS / PRODUCTS

6 Main TS							
7 Main TS							
8 Main TS							
Reboiler	Q102 Bottoms	Energy Draw	5.517e+006 * —	Liquid	10.20 *	-2.937e+005 *	107.4 *

SETUP

Sub-Flowsheet

Feed Streams			Product Streams		
Internal Stream	External Stream	Transfer Basis	Internal Stream	External Stream	Transfer Basis
Q102 Feed	Q102 @Main Feed @Main	None Req'd P-H Flash	Q101 Distillate Bottoms	Q101 @Main Distillate @Main Bottoms @Main	None Req'd P-H Flash P-H Flash

VARIABLES

Column Flowsheet Vars Available as Parameters

Data Source	Variable	Component	Description

COMPONENT MAPS

Feed Streams

Feed Name	In to SubFlowSheet	Out of SubFlowSheet
Q102 Feed		

Product Stream

Product Name	In to SubFlowSheet	Out of SubFlowSheet
Q101 Distillate Bottoms		

DYNAMICS

Vessel Dynamic Specifications

Vessel		Reboiler	Condenser	
Diameter	(m)	1.193	1.193	
Height.0	(m)	1.789	1.789	
Volume.0	(m3)	2.000 *	2.000 *	
Liquid Volume Percent	(%)	50.00 *	50.00 *	
Level Calculator		Horizontal cylinder	Horizontal cylinder	
Fraction Calculator		Use levels and nozzles	Use levels and nozzles	
Vessel Delta P	(kPa)	0.0000 *	0.0000 *	
Fixed Vessel P Spec	(kPa)	5.929	2.689	
Fixed P Spec Active		Not Active	Not Active	

Other Equipment in Column Flowsheet

Holdup Details

	Pressure (kPa)	Volume (m3)	Bulk Liquid Volume (m3)
Condenser	0.0000	0.0000 *	—

Case Name:	X:\DESKTOP\RAVIN\RAVIN.HSC
Unit Set:	SI
Date/Time:	Wed Apr 25 11:26:58 2007

UNIVERSITY OF PETROLEUM
Calgary, Alberta
CANADA

Distillation: Distillation column @Main (continued)

	Pressure (kPa)	Volume (m3)	Bulk Liquid Volume (m3)
1__Main TS	0.0000	0.0000 *	—
2__Main TS	0.0000	0.0000 *	—
3__Main TS	0.0000	0.0000 *	—
4__Main TS	0.0000	0.0000 *	—
5__Main TS	0.0000	0.0000 *	—
6__Main TS	0.0000	0.0000 *	—
7__Main TS	0.0000	0.0000 *	—
8__Main TS	0.0000	0.0000 *	—
Reboiler	0.0000	0.0000 *	—