SIMULATION & SENSITIVITY ANALYSIS OF REFORMATE SPLITTER COLUMN

A thesis submitted in partial fulfillment of the requirements for the Degree of
Master of Technology
(Refining & Petrochemical Engineering)

by

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Roll No R080207015

Under the guidance of

Dr. D.N SARAF
Distinguished Professor
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UNIVERSITY OF PETROLEUM & ENERGY STUDIES

CERTIFICATE

This is to certify that the work contained in this thesis titled **"SIMULATION & SENSITIVITY ANALYSIS OF REFORMATE SPLITTER COLUMN"** has been carried out by N.P WAJID RAHMAN (Roll No R080207015) under my supervision and has not been submitted elsewhere for a degree.

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

NOMENCLATURE

F_j = Feed entering the j^{th} stage

T_{Fj} = Temperature of the feed in j^{th} Stage

P_{Fj} = Pressure of the feed in j^{th} stage

h_{Fj} = Enthalpy of the feed in the j^{th} stage

W_j = vapour side stream

$Y_{i,j}$ = Mole Fraction in vapour phase of component i in j^{th} stage

h_{vj} = enthalpy of vapour in the j^{th} stage

T_j = Temperature of the j^{th} stage

P_j = Pressure of the j^{th} stage

L_{j-1} = liquid from above stage

$X_{i,j-1}$ = mole fraction of the liquid of component i in j-1 stage

T_{j-1} = Temperature of j-1 stage

P_{j-1} = Pressure of j-1 stage

V_{j+1} = Vapour from stage below

$Y_{i,j+1}$ = Mole fraction of vapour of component i in j+1 stage

T_{j+1} = Temperature of j+1 stage

P_{j+1} = Pressure of j+1

L_j = Liquid from stage j

U_j = Liquid side stream

X_{ij} = Mole fraction of the liquid of i component in jth stage

K_{ij} = Phase Equilibrium ratio

ABSTRACT

Reformate from Continuous Catalytic Reformer Unit (CCRU) is used to blend with Motor Sprit to increase the octane number of the same in order to meet the various standards of quality. In order to achieve the required standards, C6 and lighter ends needs to be separated from the reformate and these are send to Isomerization unit for further treating.

In this thesis a theoretical model of a Reformer Splitter column was developed which splits Reformate from CCRU into light reformate at top and heavy reformate at bottom using the plant data. The results of the model and the plant data were compared. This model was developed using PRO/II simulation software. A parametric sensitivity study was also performed on the model by varying the parameters like reflux ratio, temperature of the feed, condenser temperature, reboiler heat duty. The results were also seen when the throughput to column was increased by 10%.

Chapter 1 INTRODUCTION

Though there is more demand for diesel in our country than gasoline, the consumption of gasoline is increasing day by day. The need to produce high quality fuels have become a great challenge to refiners. With introduction of more foreign cars on our roads the demand for high quality fuels is increasing.

With respect to gasoline there are various parameters that need to be met by the refiners with respect to the quality. The quality of gasoline should be such that it should increase the performance of the vehicle engine. Hence octane number plays an important role here. Octane number is a measure of antiknock quality of the gasoline. Knocking is due to untimely burning of fuel in spark ignition engine, which result in loss of power and sometimes it is powerful enough to cause damage to engine parts. The Octane number of fuel is defined as the volume percentage of iso-octane (2,2,4-trimethyl pentane) in a blend with n-heptane which gives the same knocking characteristics as the fuel under consideration. Hence gasoline should have good octane number.

This octane number is increased by blending the gasoline pool with the reformate produced from the Continuous Catalytic Regenerating Unit. In CCR unit[1] many reactions like dehydrogenation, isomerization, dehydrocycliztion, hydrocracking take place. The reformer itself may be semi-regenerative type or continuous catalytic regenerating type. Most of the refineries are now equipped with the continuous regenerating type.

The reformate produced here basically contains benzene and its precursor compounds. These components need to be removed as there is restriction to the amount of benzene in gasoline. Hence the reformate produced is passed through a splitter column where the lighter and heavier ends splits. The lighter ends mainly consist of the C6 and lighter components and heavier fraction contains high octane reformate.

The objective of the splitter column is to split the C6 and lighter species from the heavier reformate. The overhead vapor from column is then condensed and collected. This stream is mixed with the stream from Naphtha Hydrotreating Unit and sent as feed to PENEX unit.

The Reformate from Existing CCRU feeds the Reformate Splitter above tray number 15. The feed is preheated in a Feed/bottoms exchanger. There are total of 45 trays in the column. The column is provided with a reboiler and an overhead condenser with overhead receiver. The column is equipped with valve trays. The net bottoms product at about 150°C is pumped out. The heavy bottoms product is then sent to storage to the heavy Reformate tankage and further to blending unit. The net overhead from the Reformate splitter is pumped and a portion of the Reformate splitter gross overhead is pumped back to the column as reflux.

The condenser condenses the over head vapor at 60^0C and this stream is mixed with the stream from Naphtha Hydrotreating Unit and sent as feed to PENEX unit in order to open the benzene ring. Heat is provided to the Reformate Splitter via a reboiler using medium pressure steam. The reboiler heat input is adjusted to maintain the proper reflux to feed ratio.

The top over head product should contain nearly all the lighter ends. Here the composition of the benzene plays an important role as the amount of benzene in the gasoline plays a major role. For maintaining quality standards we need to maintain the quantity of the benzene in the gasoline. Hence reformate splitter column is used to remove benzene and its precursor compounds as lighter ends in the column. This lighter ends are then taken for saturation of these compounds. This is done with the help of the isomerisation unit where all the lighter benzene precursor compounds are saturated and then send back to the blending system again.

The product obtained at the bottom should be richer in heavier compounds which increases the octane number of the gasoline. This heavier reformate is directly mixed with the gasoline in the blending system. Hence the gasoline will meet the required standard of the octane number.

The feed enters at tray number 15 at a temperature of 45^0C at pressure of 3.5 Kg/cm^2 gauge pressure. The column was operating at pressure of 2.48 Kg/cm^2 gauge pressure. The through put to the column was about 593.4 Kmol/hr. The feed will be entering in liquid phase. 88.5 Kmol/hr of lighter reformate comes out of condenser at 60^0C. The bottom heavier product from reboiler contains 504.9 Kmol/hr of heavier reformate at 153^0C.

1.1 PRESENT STUDY

A reformer splitter column which splits reformate from the Continuous Catalytic Reformer Unit into lighter reformate at the top and heavier reformate at the bottom was modeled using the available plant data. This model was developed using PRO/II simulation software. The results of the model and the plant data were compared. A parametric sensitivity analysis was also performed on the model by varying the operating parameters the results are discussed.

Chapter 2 LITERATURE

The objective of the column is to split the C6 and lighter species from the Heavier Reformate. The overhead vapor from column is then condensed and collected. This stream contains the lighter ends. The bottom stream rich in heavier components will have good octane number, and is sent to the blending unit. The lighter stream is mixed with the stream from Naphtha Hydrotreating Unit and sent as feed to PENEX unit.

There have been other investigations prior to this method. One of them like a fractional distillation column operating as gasoline splitter [2] is controlled by measuring the octane number of the column overhead fraction and adjusting the reflux to the column in response to the octane number. An octane number analyzer at the top measures the octane number and adjusts the reflux ratio accordingly to obtain the required product. The output signal of the analyzer is utilized to control reflux to maintain a given octane number in the overhead. The output signal from the octane monitor is utilized to both reset a reflux control loop, if necessary, and to offer an input signal to a blending loop which blends the overhead with varying quantities of blending stock depending on the octane number and the flow of overhead material from the column. It may be necessary in blending of the overhead produced from a gasoline splitter to know the octane number and quantity of overhead material produced since gasoline may be further used or sold on an octane barrel basis. Accordingly, the feed rate is usually, but not always, relatively constant, but it may be subject to some variation due to changes in naphtha feed composition, catalyst and/or operating conditions in either or both of the catalytic reforming unit reaction zones, or due to changes in operating conditions of the reforming unit stabilizer columns. Gasoline splitter column is maintained under operating conditions sufficient to separate the combined reformate feed stock into an overhead gasoline fraction having an end boiling point range and a bottoms fraction comprising heavy hydrocarbon constituents of the combined reformate feed having an end boiling range. The primary consideration is normally to produce an overhead fraction having an octane number of predetermined value, and this octane number is the primary control for operation of the column. Any deviation of octane number will require a compensating deviation of endpoint in order to produce an overhead product of constant octane number.

In order to accomplish the desired separation, the gasoline splitter column contains the rectification zone and the stripping zone, as indicated, in order that the most effective and efficient separation of hydrocarbon constituents may be accomplished within the fractionating column. In addition to the rectification and stripping zones, the column is provided with a reboiling section for heat input, and an overhead section which provides reflux liquid in a manner which shall be set forth hereinafter. The heavy ends of most reformate gasolines are high in octane number due to the fact that high boiling aromatic constituents are concentrated in the heavy end of the reformate.

Thus, when operating column on a reformate feed stock, any decrease in the measured octane number of the overhead product indicates that an insufficient amount of heavy boiling gasoline components is being withdrawn as a portion of the overhead product. In order to compensate for this condition, the octane monitor will call for an increase in the rectification zone temperature in order to include a greater portion of the high octane number heavy ends in the overhead vapor which leaves column. Temperature controller, being reset by the octane monitor, will then call for a decrease in reflux flow which in turn will be effected by flow controller and control valve. Again, when operating column on a reformate feed stock, an increase in the measured octane number of the overhead product is an indication that an excess of high octane number heavy ends is being withdrawn from column in the overhead fraction. The octane monitor therefore will call for a decrease in the rectification zone temperature in order to eliminate a greater portion of the heavy ends from the overhead vapor. Temperature controller being reset by the octane monitor will call for an increase in the reflux flow which in turn will be effected by flow controller and control valve.

Also along with this process there are many technologies in order to reduce the amount of benzene and benzene forming precursors in the lighter ends. Many reformer unit in India will have Naphtha Splitter Unit which splits naphtha into light naphtha and heavy naphtha. This light naphtha will contain all the lighter ends along with the harmful benzene precursor compounds. The bottom of the Naphtha Splitter unit is heavy naphtha which is free of lighter ends. This is considered as feed for the Naphtha hydrotreating unit to remove impurities. The impurities mainly consist of organic sulphur, nitrogen and oxygen. After removal of these impurities, they are taken feed to the Continuous Catalytic Reformer unit.

There is also PENNEX isomerization unit where the lighter ends are isomerized to produce high octane products. It's a part of the motor spirit quality upgradation unit. Apart from this, the liquid-liquid extraction process can be carried out in order to remove the aromatic components present in lighter ends. This can be done by extraction using glycols.

Here we consider a reformate splitter column which separates the reformate into lighter reformate and heavier reformate. This lighter reformate consists of all the lighter ends including benzene and its precursors. This overhead stream is then sent to the isomerization unit in order for further treatment. The heavier stream is then sent to the blending system for blending it with the gasoline to improve the octane number.

Chapter 3 INTRODUCTION TO SIMULATION

A model can be defined to be an abstract representation of a system usually containing structural, logical or mathematical relationships which describe a system in terms of state, entities and their attributes sets, process, events, activities and decays. However, many real world systems are so complex, that the models of these systems are virtually impossible to solve analytically. In these instances, numerical computer based simulation can be used.

Simulation is the initiation of operation of real world process or system. Simulation is considered to be the computation technique to solve problems by the observation of the performance of the dynamic model of the system. The simulation technique makes no specific attempt to involve the relationships between any particular variables instead it observes the way in which all variables of the model change with time.

Complex flowsheeting programs, that simulate the operation and a complete process, or individual units, have been developed by several commercial software organizations (see Table 3.1).

Table 3.1 Simulation Packages

Acronym	Type	Internet Address
Aspen Plus	Steady State	aspentech.com
Aspen Hysys	Steady state	hyprotech.com
Pro II	Steady state	simsci.com
CHEMCAD	Steady state	chemstations.net
UNISIM	Steady state, dynamic	honeywell.com

In this case PRO/II by Simsci was chosen as the steady state simulation tool because of its ability to quickly create a model. Steady state simulation based on first principles models is a mature technology, which is now routinely used for designing processes. Plant designs have thereby become increasingly complex, integrated and interactive.

3.1 ABOUT PRO/II

PRO/II is the flagship offering in SimSci-Esscor's Process Engineering Suite (PES). This steady-state simulator performs rigorous mass and energy balances for a wide range of processes. From oil and gas separation to reactive distillation, PRO/II combines the data resources of a large chemical component library and extensive thermodynamic property prediction methods with the most advanced and flexible unit operations techniques. Process engineers benefit from computational facilities to perform all mass and energy balance calculations needed to model most steady-state processes within the chemical, petroleum, natural gas, solids processing, and polymer industries. PRO/II runs in an interactive Windows based GUI environment. PRO/II modeling capabilities address a wide range of applications from crude oil characterization and preheating to complex reaction and separation units. The PRO/II process simulation program is designed with both the beginner and the expert in mind. It is based on a foundation of comprehensive, reliable, and accurate simulation capabilities. It is easy to use, and the input language is an extension of the universal language of chemical engineering. Expert systems, extensive input processing, and error checking allow even an inexperienced user to be instantly productive. These features have made PRO/II an industry standard.

3.2 SELECTING THERMODYNAMIC MODELS FOR PROCESS SIMULATION:

Proper selection of thermodynamic models during process simulation is absolutely necessary as a starting point for accurate process simulation. A process that is otherwise fully optimized in terms of equipment selection, configuration, and operation can be rendered essentially worthless if the process simulation is based on inaccurate thermodynamic models. Because of this, good heuristics and appropriate priority should be placed on both selecting thermodynamic models and reporting the selections in process reports.

During process simulation, thermodynamic model selection should be performed in at least two steps. Firstly, as with initial process configurations, the thermodynamic model should be chosen based on heuristics (rules of thumb) that provide for a good base case but may or may not provide the desired level of accuracy. Secondly, based on the results of the base case simulation (complete with cost estimate), improving the accuracy of the thermodynamic models should be prioritized relative to optimizing other design parameters such as the configuration of unit operations, optimization of specific unit operations, heat integration, and other degrees of freedom used to optimize processes. Optimization includes both economic and simulation accuracy aspects. Thermodynamic model definition should be revisited as often as necessary during process optimization.

EOS (Equation of state model):

EOS models calculate both liquid and vapor properties and are generally used to model systems such as LNG and cryogenic processes, mixed refrigerants, air separation, low temperature oil absorption processes, light naphtha processing, and hydrogen systems. EOS models can calculate pure, mixture, and infinite dilution properties.

Available EOS models are:

- Ideal Gas Law
- Generalized Gas law
- R-K(Redlich-Kwong)
- SRK(Soave Redlich Kwong)
- Peng Robinson

Peng-Robinson and SRK can be used to model other processes such as dehydration and crude fractionation. Both of these models also support hydrate, water freezing point, and C02 freeze out predictions.

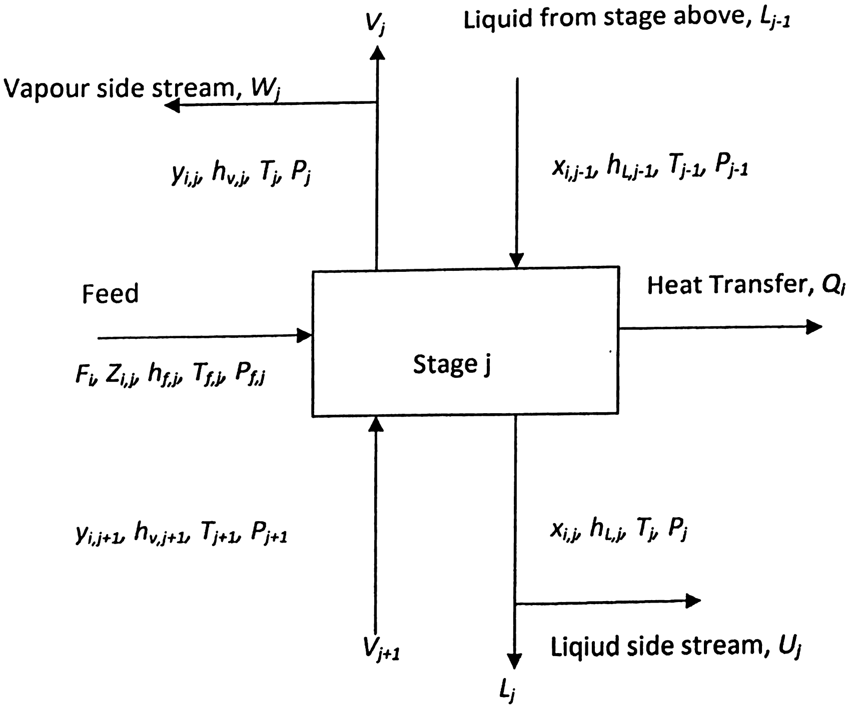
Equations of state have developed rapidly for the calculation of phase equilibria in non-polar and polar mixtures. The advantage of the equations of state method is its applicability over wide ranges of temperature and pressure to mixtures of diverse components, from the light gases to heavy liquids.

The Peng-Robinson and Soave-Redlich-Kwong equations are widely used in industry. The advantages of these equations are that they can accurately and easily represent the relation among temperature. pressure, and phase compositions in binary and multicomponent systems. They only require the critical properties and acentric factor for the generalized parameters, little computer time and lead to good phase equilibrium prediction.

Chapter 4 THEORETICAL DEVELOPMENT

A theoretical model for an equilibrium stage [3] is generated here. Consider a general, continuous, steady stage vapour –liquid or liquid-liqiud separator consisting of a number of stages arranged in a countercurrent cascade. Assume that (1) Phase equilibrium is achieved at each stage, (2)no chemical reaction occur, (3)entrainment of liquid drops in vapour and occlusion of vapour bubbles in liquid is negligible. A general representation of an equilibrium stage '*j*' is shown below for a vopor-liqiud separator where the stages are numbered from the top. The same representation applies to a liquid-liquid separator if the higher density liquid phases are represented by liquid steams and the lower density liquid phases are represented by the vapour phases.

Fig 4.1: General Equilibrium Stage



Entering stage j can be one single or two phase feed of molal flow rate F_j with overall composition in mole fraction z_{ij} of component i, temperature T_f, pressure P_f, and the corresponding overall molar enthalpy h_f. Feed pressure is assumed equal to or greater than the stage pressure P_j. Any excess feed pressure $(P_f - P_j)$ is reduced to zero adiabatically across the valve.

Leaving stage *j* is vapour of intensive properties y_{ij}, h_{vj}, T_j and P_j. This stream can be divided into a vapour side stream of molar flow rate W_j and an interstage stream of molar flow rate V_j to be sent to stage j-1 or if j=1, to leave the separator as a product. Also leaving stage *j* is liquid of intensive properties x_{ij}, h_L, T_j and P_j, which is in equilibrium with vapour (V_j+W_j). This liquid can be divided also into a liquid side stream of molar flow rate U_j and an interstage or product stream of molar flow rate L_j to be sent to stage j+1 or j=N, to leave the multistage separator as a product. Heat can be transferred at a heat Q_j from or to stage j to simulate stage intercoolers, interheaters, condensers, or reboilers.

Associated with each general theoretical stage are the following indexed equations. These equations are reffered to as MESH equations

1. *M* equations-Material balance for each component (C equations for each stage)

$$Mij=L_{j-1}x_{i,j-1} + V_{j+1,}\, y_{i,j+1} + F_j z_{i,j} - (L_j+u_j)x_{i,j} - (V_j + wj)y_i j = 0$$

2. *E* equations- Phase Equilibrium relation for each component (C equations for each stage)

$$E_{i,j} = y_{i,j} - K_{i,j}x_{i,j} = 0$$ where $K_{i,j}$ is the phase equilibrium ratio.

3. *S* equations- mole fraction summation (One for each stage)

$$(Sy)j = \sum_{i=1}^{c} Yij - 1.0 = 0$$

$$(Sx)j = \sum_{i=1}^{c} Xij - 1.0 = 0$$

4. H equations- energy balance (One for each stage)

$$H_j = L_{j-1}h_{l,j-1} + V_{j+1}h_{v,j+1} + F_jh_{Fj} - (L_j + U_j)h_{Lj} - (V_j + W_j)h_{v,j} - Q_j = 0$$

Where kinetic energy and potential energy are ignored.

Chapter 5 SIMULATION

To start with, different equipments were individually studied and was converged with the help of the tutorial data[4]. This helped basically to get a good exposure of the PRO/II and also made me aware of the possible obstacles that would come in the way during the execution of the simulation.

This project is mainly dealing with two cases:

- Simulation of the reformate splitter column with plant data
- Parametric study

The simulation of the reformate splitter column is discussed here and the parametric study is discussed in the next chapter.

The available plant data are discussed below.

COLUMN SPECIFICATIONS :

Total number of trays	:	45
Feed entering tray	:	15
Column Pressure	:	2.48 Kg/cm^2 of gauge pressure
Reboiler temperature	:	152.5 ^{0}C
Condenser temperature	:	60^{o}C
Top product flow rate	:	88 Kmol/hr
Bottom Product flow rate	:	505.41 Kmol/hr

Top tray temperature : 94^{0}C

Bottom tray temperature : 150^{0}C

FEED SPECIFICATION :

Inlet feed temperature : 45^{0}C

Inlet feed pressure : 3.5 Kg/cm^2

Flow rate : 593.41 Kmol/hr

Feed composition : the feed composition in the Table 5.1

Table 5.1 Feed composition in Kmol/hr

1)	n-Butane	:	7.22
2)	n-Pentane	:	15.8
3)	Cyclo Pentane	:	0.86
4)	2,2 DiMethyl Butane	:	2.44
5)	2,3 DiMethyl Butane	:	1.32
6)	2 Methyl Pentane	:	11.14
7)	3 Methyl Pentane	:	8.08
8)	n-Hexane	:	8.36
9)	Methyl Cyclo Pentane	:	0.71
10)	Benzene	:	26.88
11)	2,2 DiMethyl Pentane	:	1.32
12)	2,3 DiMethyl Pentane	:	41.5
13)	2,4 DiMethyl Pentane	:	7.72
14)	3,3 DiMethyl Pentane	:	2.15
15)	n-Heptane	:	20.96
16)	Methyl Cyclo Hexane	:	0.61

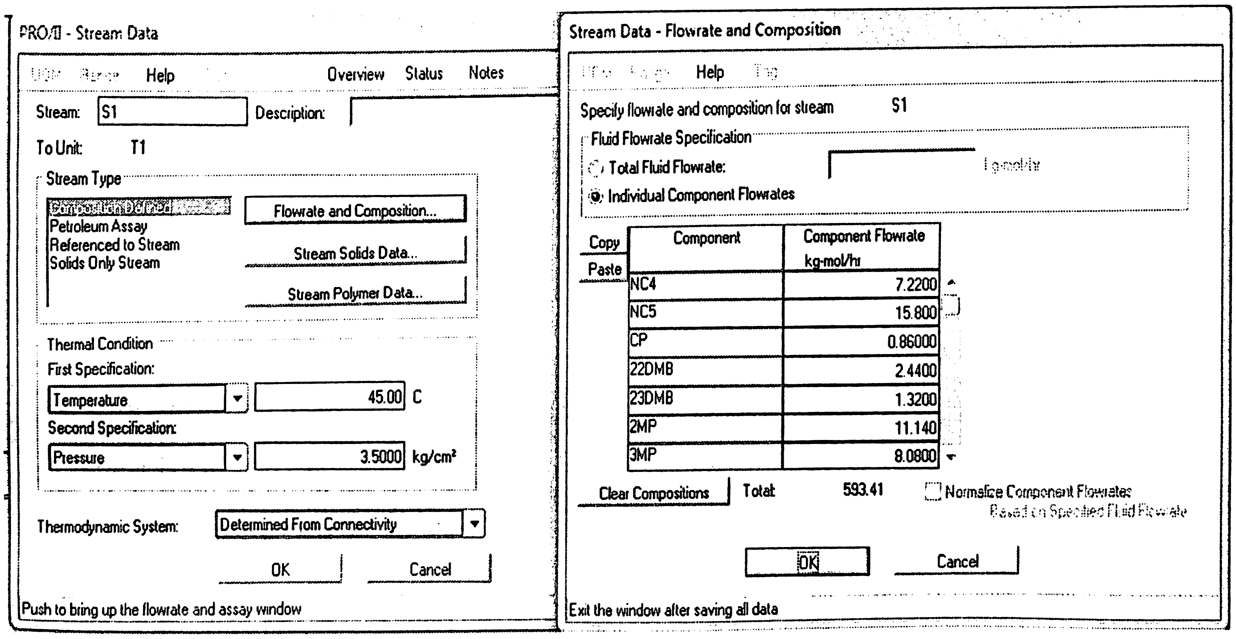
17) Toluene	:	139.35
18) n-Octane	:	296.99

593.41 Kmol/hr

The objective is to obtain C6 and lighter components in the top and heavier components at the top. The obtained output flow rate from plant for top product is 88 Kmol/hr and for heavy product is 505.41 Kmol/hr. Along with this the bottom should contain less amount of benzene and more of higher ends.

TO SIMULATE THE SPLITTER COLUMN.

The simulation is first started with opening the simulation window as shown in Fig 5.1 and start entering the component and flow rate from the above table. Along with this any critical parameters of the feed like temperature and pressure is also added. Either total flow rate is added and mole fraction can be given for each compound or individual component flow rates may be given.



Stream: S1

Description:

To Unit: T1

First Specification: Temperature 45.00 C

Second Specification: Pressure 3.5000 kg/cm²

Thermodynamic System: Determined From Connectivity

Push to bring up the flowrate and assay window

Specify flowrate and composition for stream S1

○ Total Fluid Flowrate: kg-mol/hr

● Individual Component Flowrates

Component	Component Flowrate kg-mol/hr
NC4	7.2200
NC5	15.800
CP	0.86000
22DMB	2.4400
23DMB	1.3200
2MP	11.140
3MP	8.0800

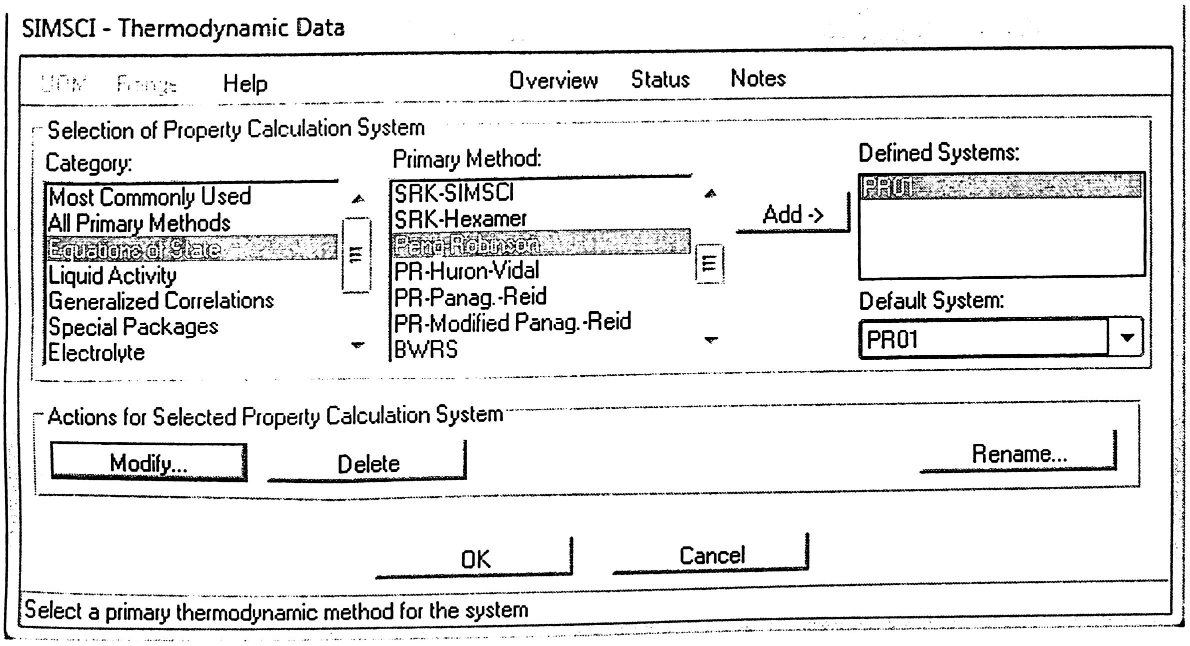
Total: 593.41

☐ Normalize Component Flowrates Based on Specified Fluid Flowrate

Exit the window after saving all data

Fig-5.1: Entering the Components

After choosing the components the required fluid package or thermodynamic data is selected as shown in Fig 5.2. Many numbers of fluid packages are available and we choose Peng-Robinson as it is more apt for refinery distillation process.



Category: Equations of State

Primary Method: Peng-Robinson

Defined Systems: PR01

Default System: PR01

Select a primary thermodynamic method for the system

Fig 5.2: Fluid package selection

After selection of required thermodynamic data and the component, we select the required unit from the Process Flow Diagram Palette. Here we select a column with 45 trays including condenser and reboiler. After selecting the column, we connect our feed stream to it. The PRO/II platform window is shown in Fig 5.3

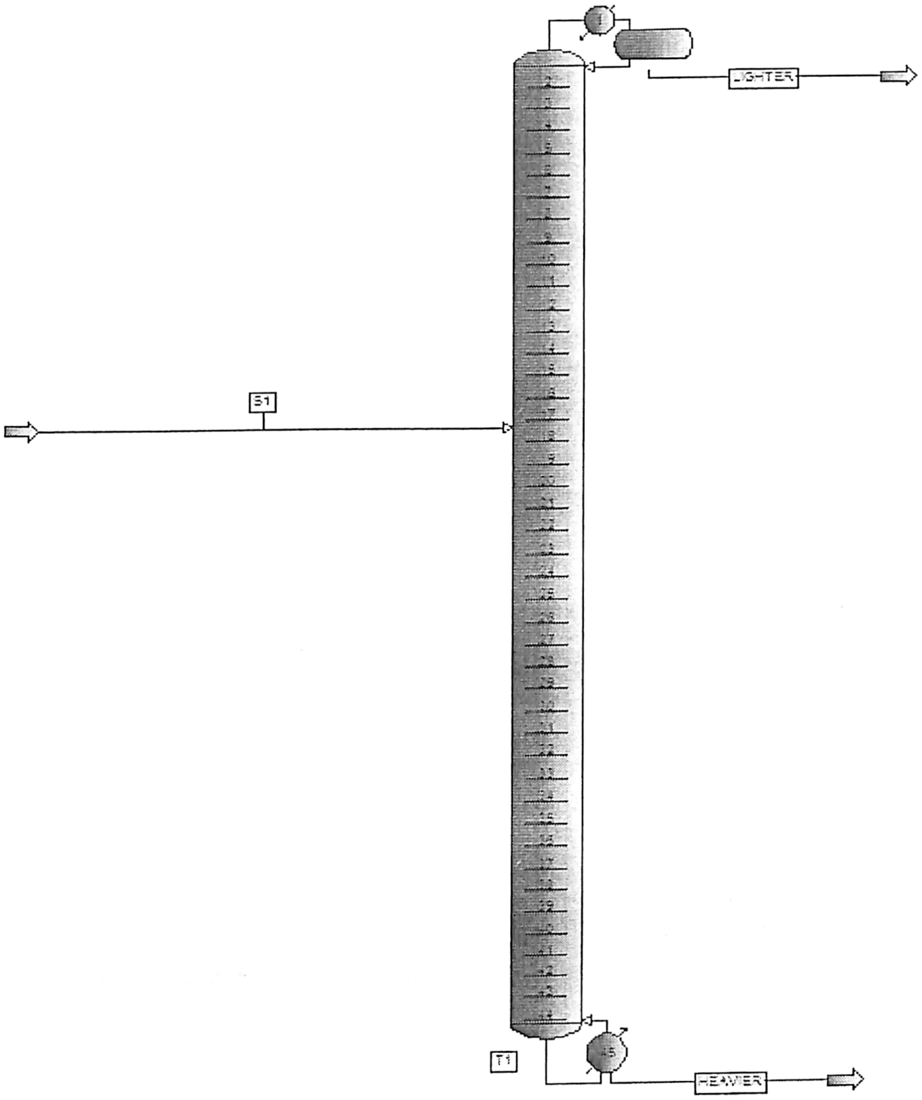
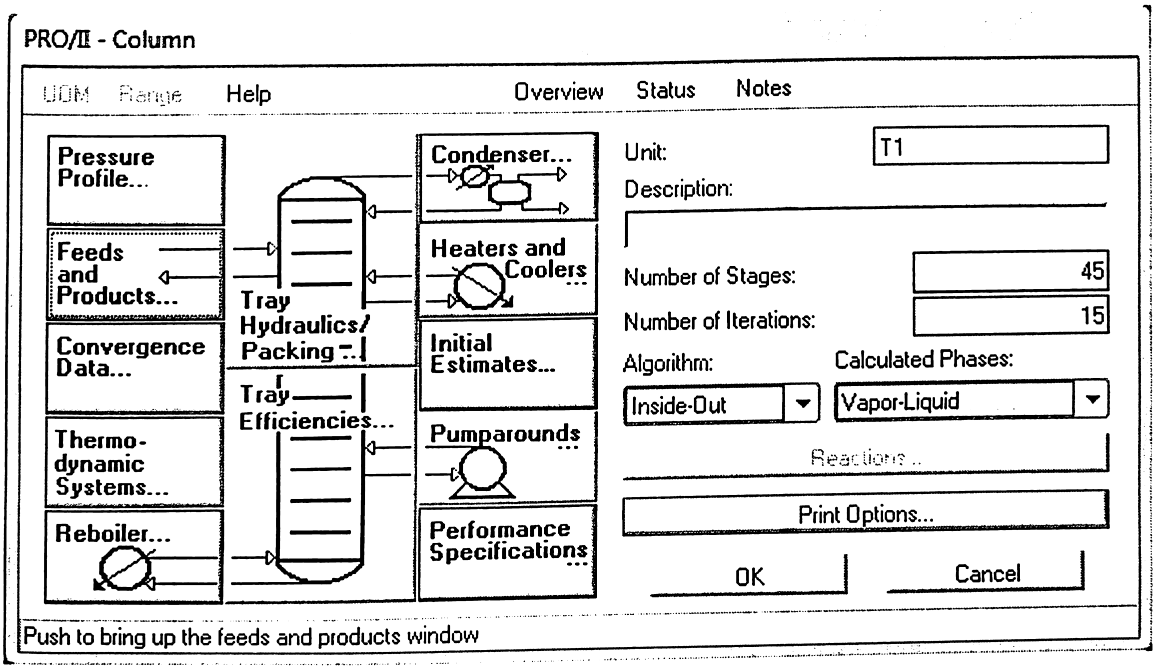


Fig 5.3: Reformer Splitter Column

On double clicking the column we get the whole details about the column. We could enter any data by clicking the required tab as shown in Fig 5.4. For example we click on the pressure profile tab to enter the pressure details. Similarly feed entering tray details is also entered through here and also we enter the condenser and reboiler data.



PRO/II - Column

Unit: T1

Description:

Number of Stages: 45

Number of Iterations: 15

Algorithm: Inside-Out

Calculated Phases: Vapor-Liquid

Push to bring up the feeds and products window

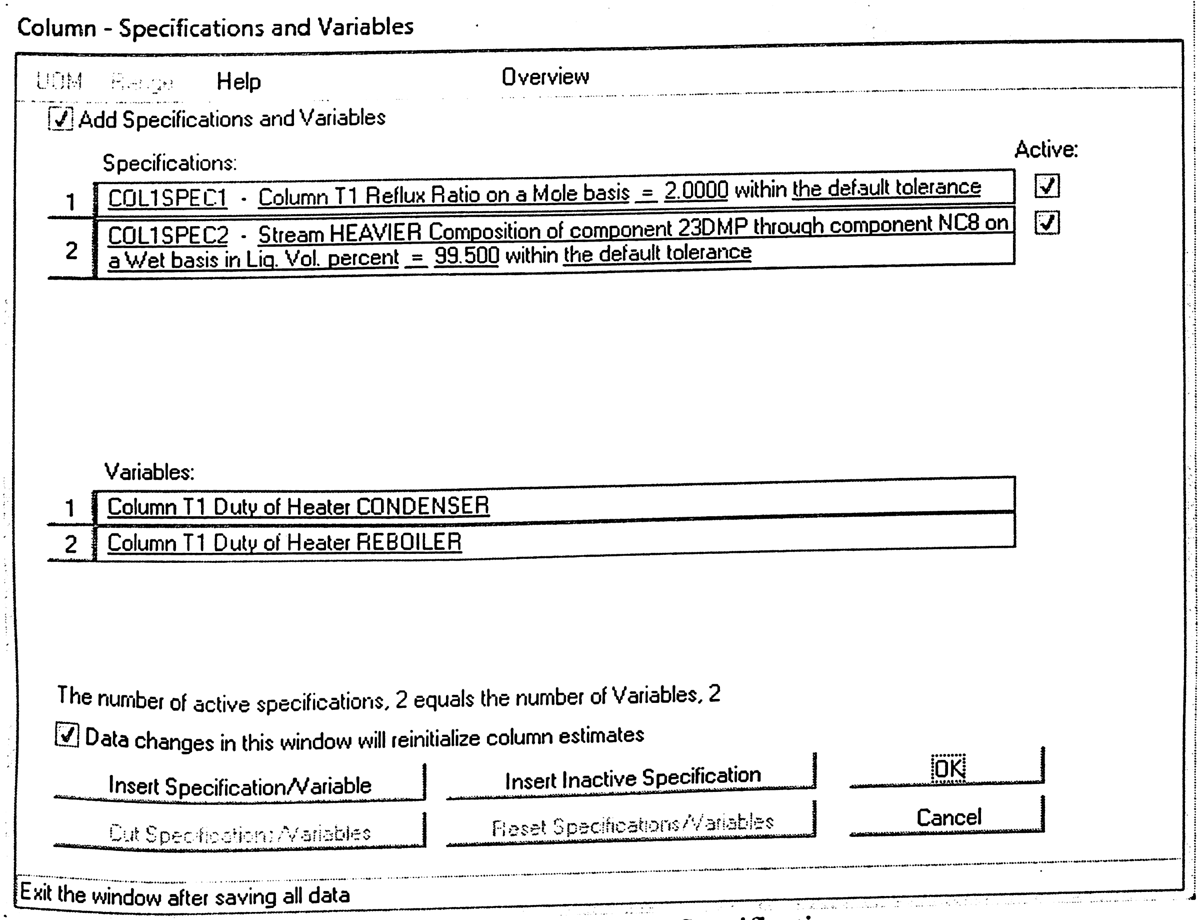
Fig 5.4 : Splitter column entry

One of the key aspects here is performance specification. Here the simulator allows us to enter any required specification so that it simulates according to the specification given by the user. Any required specification can be given here along with the required variable.

Here we give two specification along with two variables. The following specifications are given here

- The column Reflux Ratio on mole basis = 2.00
- The bottom heavier reformate composition of last five component in liquid volume percent = 99.5

This specification is entered as shown in Fig 5.5 and by giving this specification we simulated the plant data to match output of simulator with the output of the plant. Later even in performance study analysis also, we kept this performance specification as same and then simulated to find the output.



Specifications:

1 COL1SPEC1 - Column T1 Reflux Ratio on a Mole basis = 2.0000 within the default tolerance ☑

2 COL1SPEC2 - Stream HEAVIER Composition of component 23DMP through component NC8 on a Wet basis in Liq. Vol. percent = 99.500 within the default tolerance ☑

Variables:

1 Column T1 Duty of Heater CONDENSER

2 Column T1 Duty of Heater REBOILER

The number of active specifications, 2 equals the number of Variables, 2

☑ Data changes in this window will reinitialize column estimates

Exit the window after saving all data

Fig 5.5: Column Performance Specifications

With the above given values we start to the run the software to get the required output as that of plant. The run button from the toolbar is clicked and the programme runs the values and provides the required output values. We can also add stream property tables to the working environment for better understanding of the column like we can add component composition table or flow rate table so as to easily view the require changes in output. Similarly any tables can be made there by reducing the time by generating the report and then checking it.

In this way the base case model is generated and the output of it is compared with the plant output. The parametric sensitivity study by changing the various parameters of this base case model is been discussed in the following chapters.

Chapter 6 RESULTS AND DISCUSSIONS

The model is developed for the given plant data of the reformate splitter column and a sensitivity analysis was performed for the model. From the obtained output we incur the following results.

6.1 Simulation of the Reformate Splitter Column

From the given plant data of the reformate splitter column, we simulated it using PRO/II simulator software to obtain the desired output. This output was then compared with the original plant data. The original plant output data consist of the following

Output flow rate:

Light Reformate Flow rate: 88 Kmol/hr

Heavy reformate Flow rate: 505.41 Kmol/hr

The product composition is given in Table 6.1

Serial No:	Component Name	Lighter Reformate Kmol/hr	Heavier Reformate Kmol/hr
1.	n-Butane	7.22	-
2.	n-Pentane	15.8	-
3.	Cyclo Pentane	0.8597	0.0002
4.	2,2 DiMethyl Butane	2.4387	0.0012
5.	2,3 DiMethyl Butane	1.3112	0.0087
6.	2 Methyl Pentane	11.0549	0.08505
7.	3 Methyl Pentane	7.8939	0.1860
8.	n-Hexane	7.7525	0.6074
9.	Methyl Cyclo Pentane	0.5748	0.1351
10.	Benzene	23.1706	3.7093
11.	2,2 DiMethyl Pentane	0.7576	0.5623
12.	2,3 DiMethyl Pentane	6.8962	34.6037
13.	2,4 DiMethyl Pentane	4.2101	3.5098

14.	3,3 DiMethyl Pentane	0.5892	1.5607
15.	n-Heptane	0.4887	20.4712
16.	Methyl Cyclo Hexane	0.0037	0.6062
17.	Toluene	0.1065	139.2434
18.	n-Octane	0.00029	296.9896

Table 6.1: Plant output component composition

This plant output composition was then compared to simulated output generated by the simulator. The output that was generated by the simulator is given by the following table. The detailed output generated can be viewed in the annexure.

Serial No:	Component Name	Lighter Reformate, Kmol/hr	Heavier Reformate, Kmol/hr	Feed, Kmol/hr
1.	n-Butane	7.22	-	7.2200
2.	n-Pentane	15.8	2.6583 E-11	15.8800
3.	Cyclo Pentane	0.8600	4.5735 E-09	0.8600
4.	2,2 DiMethyl Butane	2.4400	6.7305 E-08	2.4400
5.	2,3 DiMethyl Butane	1.3200	8.2894 E-06	1.3200
6.	2 Methyl Pentane	11.1399	8.4909 E-05	11.1400
7.	3 Methyl Pentane	8.0791	9.0228E-04	8.0800
8.	n-Hexane	8.3436	0.0164	8.3600
9.	Methyl Cyclo Pentane	0.6873	0.0227	0.7100
10.	Benzene	23.7753	3.1047	26.8800
11.	2,2 DiMethyl Pentane	0.7593	0.5607	1.3200
12.	2,3 DiMethyl Pentane	3.4823	38.0177	41.5000
13.	2,4 DiMethyl Pentane	4.0378	3.6822	7.7200
14.	3,3 DiMethyl Pentane	0.3541	1.7959	2.1500
15.	n-Heptane	0.1694	20.7906	20.9600
16.	Methyl Cyclo Hexane	1.4482E-03	0.6086	0.6100
17.	Toluene	0.0288	139.3213	139.3500
18.	n-Octane	9.2932E-05	296.9896	296.9900

Table 6.2: Simulator output component composition

	Lighter Reformate	Heavier reformate	Feed
Total Rate, Kmol/Hr	88.4985	504.9115	593.4100
Temperature, ^{0}C	60.0000	152.8962	45.0000
Pressure, Kg/cm^2	2.4500	2.7800	3.5000
Enthalpy, M Kcal/Hr	0.2344	4.5595	1.5021
Molecular weight	80.4437	106.0902	102.2654

From the above table it is clear that the output of the model generated by the simulator is almost matching with the plant data. Even the flow rate of the plant is matching. Hence the base case model is obtained. Here again the specification given was reflux ratio and the bottom component composition. With this specification we get the required output.

A plot was generated between the tray number and flow rates of liquid, vapour and temperature (see Fig 6.1). From the plot it is evident that as the tray number increases the liquid rate increases. Similarly the temperature has a maximum at the bottom. The vapour rate is comparatively less at the bottom.

This model generated is basically considered as the base case model and the parametric sensitivity analysis is done on this model

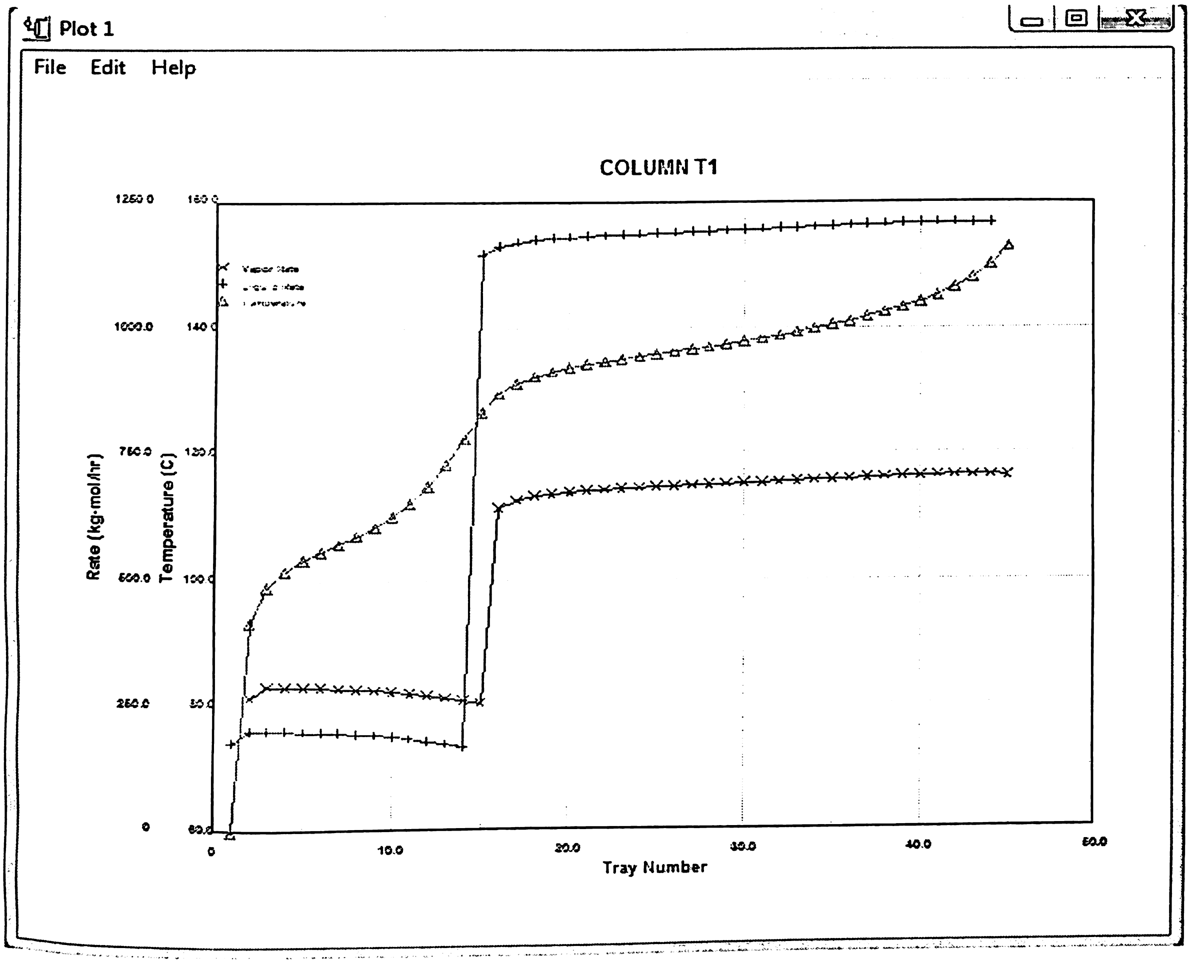


Fig 6.1: Plot between tray number and flow rates of liquid, vapour and temperature

Chapter 7 PARAMETRIC SENSITIVITY ANALYSIS

A detailed parametric sensitivity analysis is done on the base case model by changing various operating parameters. The behaviour of the model by changing the parameters is then studied. Only one variable was disturbed at a time and all other specification remained the same. Even the performance specification was not altered. By varying the parameters we could obtain how the model react to change in parameters and also to obtain the optimized operating conditions.

The various parameters that we changed are

- Temperature of the feed increased and decreased by 10%
- Condenser temperature increased and decreased by 10%
- Reflux ratio increased and decreased by 10%
- Reboiler temperature increased to 153.4^{0}C
- Reboiler heat duty increased to 5.75 MKcal/Hr
- Increasing the feed flow rate by 10%

The output that is obtained each time is compared with base model output. By this way the optimized model is provided for maximum recovery of benzene at the top of the column and heavier components at the bottom.

7.1 Temperature of the feed

The temperature of the feed is 45^{0}C for the base case model. This temperature is then increased and decreased by around 10%. Hence the study is performed on the base case model by changing the temperature to 40^{0}C and to 50^{0}C. The temperature of the feed is changed and the model is made to run in the simulator to study the variations from the base case. Here only the feed temperature is changed and all other conditions and specifications remains the same as that of the base case. When the temperature is being changed from the original feed temperature, difference in the flow rate of the products and the heat duties is noted. There is a change in the heat duty of the condenser and reboiler. Also a slight change in the product composition is also noted.

With change in temperature of the feed, we obtain the following result which is compared with the base case model.

Properties	Output at Temperature 40^{0}C	Output at Temperature 50^{0}C	Base case output model
Lighter Reformate flow rate, Kmol/Hr	87.9	89.2	88.5
Heavier Reformate flow rate, Kmol/Hr	505.5	504.2	504.9
Condenser Duty, MKcal/Hr	-2.0054	-2.0450	-2.0236
Reboiler Duty, MKcal/Hr	5.4480	5.1835	5.3153

Table 7.1: Output at different temperature of feed

Apart from the above mentioned changes, there is an elementary change in the product component composition with the flow rate. From the above output it is clear that reducing or increasing the temperature of the feed has a little effect on the output produced. Hence they are recommended for the cost beneficial purpose as it reduces the heat duties of condenser and reboiler.

7.2 Condenser Temperature

The temperature of the condenser is changed by 10% from the original base case model. The temperature of condenser in base case model is about 60^0C. This temperature is then varied to 54^0C and to 66^0C. The model is made to run with changed temperature of the condenser and the output was generated. The output is then compared with the output of the base case model. Here only the temperature of the condenser is changed and all other conditions and specifications remains the same as that of the base model. When the temperature of condenser is being changed from the original condenser temperature, difference in the flow rate of the products and the heat duties is noted. There is a change in the heat duty of the condenser and reboiler as that of the original model data. Also a slight change in the product composition is also noted. With change in condenser temperature we obtain the following results which are compared with the base case model.

Properties	Output at condenser Temperature 54^0C	Output at condenser Temperature 66^0C	Base case output model
Lighter Reformate flow rate, Kmol/Hr	88.0	89.1	88.5
Heavier Reformate flow rate, Kmol/Hr	505.4	504.4	504.9
Condenser Duty, MKcal/Hr	-2.0742	-1.9729	-2.0236
Reboiler Duty, MKcal/Hr	5.3456	5.2854	5.3153

Table 7.2: Output at different condenser temperature

Apart from the above mentioned changes, the product component composition also changes slightly along with flow rate of the product. From the above output it is clear that reducing or increasing the temperature of the condenser has a little effect on the output produced and also its component composition.

7.3 Reflux Ratio

The reflux ratio of the column is increased and decreased by 10% from the original value. The reflux ratio of the original base model was 2.00. This reflux ratio was modified to 1.8 and 2.2. With change in reflux ratio the model is the simulated to get the output. Here only the reflux ratio is being changed and all other specifications remain the same. The simulated output is then compared with the output of the base model. With change in the reflux ratios slight change in flow rate of products and the heat duties of the condenser and reboiler is noticed. Also a small change in individual component composition is also seen in the output that was obtained. With change in reflux ratio we obtain the following results which are compared with the base case model.

Properties	Output at Reflux Ratio = 1.8000	Output at Reflux Ratio = 2.2000	Base case output model
Lighter Reformate flow rate, Kmol/Hr	90.3	87.2	88.5
Heavier Reformate flow rate, Kmol/Hr	503.1	506.2	504.9
Condenser Duty, MKcal/Hr	-1.9430	-2.1140	-2.0236
Reboiler Duty, MKcal/Hr	5.2282	5.4103	5.3153

Table 7.3: Output at different reflux ratio

Apart from the above mentioned output changes the product composition also changes. For decrease in reflux ratio to 1.8000, marginal increase in the top product is obtained. Hence the duty of the condenser is reduced. Similarly with increase in reflux ratio the heavier product is increased. A better recovery of the bottom product is seen here at the increased reflux ratio. The bottom component like 2,3 di methyl pentane is recovered more.

7.4 Reboiler Temperature:

The Reboiler temperature of the base case model is about 152.9^{0}C. The reboiler temperature is then increased to 153.4^{0}C. The model is then simulated with this increased reboiler temperature and output was compared with the base model output. Apart from the changes obtained from the heat duties of condenser and reboiler, the product component composition is also varied here. The following results have been obtained.

Properties	Output at Reboiler temp of 153.4^{0}C	Base case output model
Lighter Reformate flow rate, Kmol/Hr	93.5	88.5
Heavier Reformate flow rate, Kmol/Hr	499.9	504.9
Condenser Duty, MKcal/Hr	-2.1641	-2.0236
Reboiler Duty, MKcal/Hr	5.4489	5.3153
Benzene composition in Lighter Reformate, Kmol/Hr	25.8401	23.7753
Benzene composition in heavier Reformate, Kmol/Hr	1.0399	3.1047

Table 7.4: Output at increased Reboiler temperature

With the increase in the reboiler temperature the flow rate of the top lighter ends has increased. From the output it is clear that the amount of the top product has increased than original model. There is a significant increase in the amount of the benzene in the top composition. Hence with increase in reboiler temperature the amount of benzene content increases in top lighter end which is an optimize condition. Hence better recovery of bottom product is also obtained. Therefore this is an apt condition for maximization of the products.

7.5 Reboiler Heat Duty:

The Reboiler heat duty of the column was increased to 5.75 MKcal/Hr from 5.315 MKcal/Hr. The model is then simulated with this increased reboiler heat duty and output was compared with the base case model output. With increase in the reboiler heat duty a change in product flow rate and individual component composition is obtained. The optimized model is then generated here with increase in the reboiler heat duty. This increase in the reboiler heat duty increases the reboiler temperature there by increasing the yield of the top product ie lighter reformates. The output of the model is compared with the base model below.

Properties	Output at reboiler duty of 5.75 MKcal/Hr	Base case model output
Lighter Reformate flow rate, Kmol/Hr	104.4	88.5
Heavier Reformate flow rate, Kmol/Hr	489.0	504.9
Condenser Duty, MKcal/Hr	-2.4965	-2.0236
Reboiler Duty, MKcal	5.75	5.3153

Benzene composition in lighter reformate, Kmol/hr	26.8073	23.7753
Benzene composition in heavier reformate, Kmol/hr	0.0727	3.1047

Table 7.5: Output at increased reboiler heat duty

The increase in reboiler heat duty increases the reboiler temperature thereby causing a better recovery of the lighter ends. Hence the benzene composition is comparatively less in the heavier stream. More benzene is recovered in the lighter stream.

7.6 Increased Feed Flow rate

The through put to the column is increased by 10% and then the model is then studied. Only the through put to the column is increased. All the remaining parameters remain the same as of that of the base model. The feed rate is increased from 593.4 Kmol/Hr to 652.7 Kmol/Hr. With this increase in feed flow rate the model is obtained with optimized operating condition. Apart from the change in the heat duties of the condenser and the reboiler, the individual component composition is also varied from the output of the base model.

The simulated output for the increased feed flow rate is determined and is compared with the base model below.

Properties	Output at throughput of 652.7, Kmol/Hr	Plant Data
Lighter Reformate flow rate, Kmol/Hr	102.8	88.5
Heavier Reformate flowrate, Kmol/Hr	549.9	504.9
Condenser Duty, MKcal/Hr	-2.3809	-2.0236
Reboiler Duty, MKcal/Hr	5.9948	5.3153

Table 7.6: Output at increased feed flow rate

Apart from the above output, the composition of the component also changes. Here we get a good recovery of the top lighter ends. This is because the increase in the through put increases the reboiler heat duty which simultaneously increases the reboiler temperature. This increase in reboiler temperature shows a better yield of the products.

Chapter 8 CONCLUSION

A reformate splitter column has been simulated on PRO/II platform. The calculated flow rates, temperatures and compositions match well with the plant data. Using this model, a parametric sensitivity study was undertaken in which variations up to 10% increase and decrease were provided in parameters like temperature of feed, condenser temperature, reflux ratio, reboiler heat duty and their effects studied on the splitter column performance. Also optimized condition for 10% increase in throughput has been generated.

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4. PRO/ii V 8.0 User's Guide

ANNEXURE-I : The output generated by PRO/II for the base case model.

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SIMULATION SCIENCES INC.           R                                  PAGE P-4
PROJECT                        PRO/II  VERSION 8.0 ELEC V6.6
PROBLEM                                    OUTPUT
                                       COLUMN SUMMARY                 04/17/09
==============================================================================

                                  UNIT 2, 'T1'

TOTAL NUMBER OF ITERATIONS

    IN/OUT METHOD       12

COLUMN SUMMARY

                                  ---------- NET FLOW RATES -----------      HEATER
 TRAY    TEMP   PRESSURE    LIQUID    VAPOR     FEED     PRODUCT       DUTIES
        DEG C   KG/CM2                  KG-MOL/HR                      M*KCAL/HR
------ ------- --------  -------- -------- --------- ---------   ------------
    1C   60.0     2.45      177.0                                88.5L      -2.0236
     2   93.3     2.48      199.2    265.5
     3   99.0     2.49      199.2    287.7
     4  101.7     2.49      198.3    287.7
     5  103.4     2.50      197.3    286.8
     6  104.7     2.51      196.2    285.8
     7  105.9     2.51      195.0    284.7
     8  107.1     2.52      193.4    283.5
     9  108.5     2.53      191.3    281.9
    10  110.2     2.54      188.6    279.8
    11  112.2     2.54      184.9    277.1
    12  114.9     2.55      180.3    273.4
    13  118.3     2.56      175.2    268.8
    14  122.3     2.56      170.1    263.7
    15  126.5     2.57     1147.8    258.6     593.4L
    16  129.6     2.58     1163.0    642.8
    17  131.2     2.58     1170.5    658.1
    18  132.3     2.59     1174.9    665.6
    19  133.1     2.60     1177.9    670.0
    20  133.7     2.61     1180.2    673.0
    21  134.2     2.61     1182.2    675.3
    22  134.7     2.62     1183.8    677.2
    23  135.1     2.63     1185.3    678.9
    24  135.5     2.63     1186.7    680.4
    25  135.9     2.64     1188.1    681.8
    26  136.3     2.65     1189.4    683.2
    27  136.6     2.65     1190.7    684.5
    28  137.0     2.66     1192.0    685.8
    29  137.4     2.67     1193.3    687.0
    30  137.9     2.68     1194.6    688.3
    31  138.3     2.68     1196.0    689.7
    32  138.8     2.69     1197.4    691.0
    33  139.4     2.70     1198.8    692.4
    34  139.9     2.70     1200.3    693.9
    35  140.5     2.71     1201.7    695.3
    36  141.1     2.72     1203.2    696.8
    37  141.8     2.72     1204.6    698.3
    38  142.5     2.73     1206.0    699.7
    39  143.3     2.74     1207.2    701.1
    40  144.2     2.75     1208.2    702.3
    41  145.2     2.75     1208.8    703.3
```

```
  42     146.4      2.76    1209.0    703.9
  43     148.0      2.77    1208.4    704.0
  44     150.1      2.77    1207.1    703.5
  45R    152.9      2.78              702.2                  504.9L         5.3153

 FEED AND PRODUCT STREAMS

  TYPE      STREAM      PHASE     FROM  TO    LIQUID          FLOW RATES     HEAT RATES
                                  TRAY  TRAY   FRAC           KG-MOL/HR      M*KCAL/HR
  ----- ------------ ------     ----  ----  ------        ------------   ------------
  FEED  S1           LIQUID            15   1.0000              593.41         1.5021
  PROD  LIGHTER      LIQUID        1                             88.50         0.2344
  PROD  HEAVIER      LIQUID       45                            504.91         4.5595

  OVERALL MOLE BALANCE, (FEEDS - PRODUCTS)                       0.00
  OVERALL HEAT BALANCE, (H(IN) - H(OUT)  )                                5.0207E-06

 SPECIFICATIONS

  SPECIFICATION   PARAMETER   TRAY    COMP    SPECIFICATION   SPECIFIED    CALCULATED
     NUMBER         TYPE       NO      NO          TYPE          VALUE        VALUE
  -------------   ---------   ----   ------   -------------   ----------   ----------
    1 (ACTIVE)    UNIT T1       1             MOL RRATIO      2.000E+00    2.000E+00
    2 (ACTIVE)    STRM HEAV    45    12- 18   LV  PERCENT     9.950E+01    9.950E+01
    3 (INACTIVE)  STRM LIGH     1             MOL RATE        8.800E+01    8.850E+01

 REFLUX RATIOS

                                           -------- REFLUX RATIOS --------
                                             MOLAR      WEIGHT    STD L VOL
                                           ---------  ---------  ---------
  REFLUX / FEED STREAM S1                    0.2983     0.2346     0.2459
  REFLUX / LIQUID DISTILLATE                 2.0000     2.0000     2.0000

SIMULATION SCIENCES INC.              R                                  PAGE P-9
PROJECT                          PRO/II  VERSION 8.0 ELEC V6.6
PROBLEM                                     OUTPUT                       04/17/09
==============================STREAM MOLAR COMPONENT RATES=======================

 STREAM ID                                 HEAVIER       LIGHTER           S1
        NAME                                             lighter
        PHASE                              LIQUID        LIQUID         LIQUID
  THERMO ID                                  PR01          PR01           PR01

 FLUID RATES, KG-MOL/HR
  1  NC4                                   0.0000        7.2200         7.2200
  2  NC5                               2.6583E-11       15.8000        15.8000
  3  CP                                4.5735E-09        0.8600         0.8600
  4  22DMB                             6.7305E-08        2.4400         2.4400
  5  23DMB                             8.2894E-06        1.3200         1.3200
  6  2MP                               8.4909E-05       11.1399        11.1400
  7  3MP                               9.0228E-04        8.0791         8.0800
  8  NC6                                   0.0164        8.3436         8.3600
  9  MCP                                   0.0227        0.6873         0.7100
 10  BNZN                                  3.1047       23.7753        26.8800
 11  22DMP                                 0.5607        0.7593         1.3200
 12  23DMP                                38.0177        3.4823        41.5000
 13  24DMP                                 3.6822        4.0378         7.7200
```

```
   14  33DMP                         1.7959      0.3541       2.1500
   15  NC7                          20.7906      0.1694      20.9600
   16  MCH                           0.6086  1.4482E-03       0.6100
   17  TOLUENE                     139.3213      0.0288     139.3500
   18  NC8                         296.9899  9.2932E-05     296.9900

 TOTAL RATE, KG-MOL/HR             504.9115     88.4985     593.4100

 TEMPERATURE, C                    152.8962     60.0000      45.0000
 PRESSURE, KG/CM2                    2.7800      2.4500       3.5000
 ENTHALPY, M*KCAL/HR                 4.5595      0.2344       1.5021
 MOLECULAR WEIGHT                  106.0902     80.4437     102.2654
 MOLE FRAC VAPOR                     0.0000      0.0000       0.0000
 MOLE FRAC LIQUID                    1.0000      1.0000       1.0000
□
```