

**MODELING & SIMULATION OF PROPYLENE/PROPANE
FRACTIONATOR (C₃ SPLITTER)
USING ASPEN HYSYS**

**A PROJECT REPORT SUBMITTED IN PARTIAL FULFILLMENT OF
THE REQUIREMENTS FOR THE DEGREE OF**

MASTER OF TECHNOLOGY

IN

**Refining & Petrochemical Engineering
(ACADEMIC SESSION: 2005-2007)**

BY

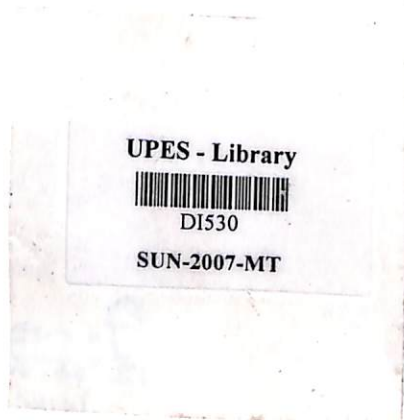
RAM KUMAR SUNDARAPU

Roll No: R080205015

UNDER THE SUPERVISION OF

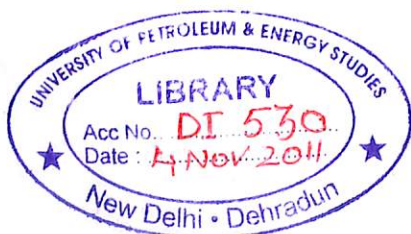
Dr. D.N. Saraf

(Distinguished professor)



**College Of Engineering,
University of Petroleum & Energy Studies,
Dehradun (U.A.)**

May 2007





UNIVERSITY OF PETROLEUM & ENERGY STUDIES

CERTIFICATE

This is to certify that the project work entitled “**Modeling & Simulation of Propylene/Propane Fractionator(C₃ Splitter) using ASPEN HYSYS**” submitted by Mr.Ram Kumar Sundarapu in partial fulfillment of the requirements for the degree of Master Of Technology (Refining & Petrochemical Engineering), at college of engineering, University of Petroleum and Energy Studies, is a record of the work carried by him at UPES, Dehradun under the guidance of “Dr.D.N.Saraf, Distinguished Professor, COE, UPES” .

To the best of my knowledge, the contents of this project work did not form a basis of the award of any previous degree or published material by any one else.



14.02.07

Dr.D.N.Saraf

Professor, COE

UPES

Dehradun


14/05/07

Dr. B. P. Pandey

Dean, COE

UPES

Dehradun

Corporate Office :
Hydrocarbons Education & Research Society
1st Floor, PHD House 4/2, Siri Institutional Area
August Kranti Marg, New Delhi-11001 India
Ph + 91-11-41730151-53 Fax +91-11 1730154

Main Campus :
Energy Acres, PO Bidholi, Via Prem Nagar,
Dehradun-248 007 (Uttaranchal) India
Ph. +91-135-2261090-91, 2694201/203/208
Fax +91-135-2694204

Regional Centre (NCR) :
SCO 9-12, Sector-14, Gurgaon 122 007
(Haryana), India
Ph + 91-124-4540300
Fax +91 124 4540 330



UNIVERSITY OF PETROLEUM & ENERGY STUDIES

CERTIFICATE

This is to certify that the work contained in this thesis entitled “**Modeling and Simulation of Propylene/Propane fractionator (C₃ Splitter) using ASPEN HYSYS**” has been carried out by Mr. Ram Kumar Sundarapu under my supervision and that this work has not been submitted elsewhere for a degree.

D.N. Saraf
14.08.07

Dr. D.N. Saraf,
Distinguished professor,
College of Engineering,
University of petroleum and Energy Studies,
Dehradun – 248007.

Corporate Office :
Hydrocarbons Education & Research Society
1st Floor, PHD House 4/2, Siri Institutional Area
August Kranti Marg, New Delhi-11001 India
Ph + 91-11-41730151-53 Fax +91-11 1730154

Main Campus :
Energy Acres, PO Bidholi, Via Prem Nagar,
Dehradun-248 007 (Uttaranchal) India
Ph. +91-135-2261090-91, 2694201/203/208
Fax : +91-135-2694204

Regional Centre (NCR) :
SCO 9-12, Sector-14, Gurgaon 122 007
(Haryana), India
Ph + 91-124-4540300
Fax +91 124 4540 330

E-mail : info@upes.ac.in URL www.upes.ac.in

ACKNOWLEDGEMENT

This is to acknowledge with thanks the help, guidance and the support that I have received during my project work.

I avail this opportunity to place our profound sense of gratitude to our project guide Dr. D.N. Saraf, Distinguished professor of college of engineering, UPES, Dehradun for giving his valuable advice and guidance to pursue my project.

I am very much thankful to Mr. M.A. Subramanian (General Manager), Mr. J.N Shah (DGM), GOP and Team of Naptha Cracker plant of IPCL (Indian Petrochemicals Corporation Limited, Vadodara complex) in allotting a valuable project & extended their co-operation throughout my project work.

I also express my sincere gratitude to Mr. T.Chandrasekhar, lecturer of college of engineering, UPES, Dehradun for his guidance right from the beginning of the investigation to its completion.

I am immensely indebted to my parents, who have always rendered their support and helped me to complete this project successfully.

I also place on record my recognition of the support provided by my colleagues, team of UPES during the completion of this project.

Ram Kumar
14/05/06

Ram Kumar Sundarapu

M.Tech (Refining & Petrochemical Engineering)

Roll No. R080205015

UPES, Dehradun.

Email ID: ramkumar034@gmail.com

CONTENTS

List of tables

List of flow sheets

List of charts

List of plots

| | |
|---|--------------|
| Chapter 1: Introduction | 1-6 |
| 1.1 Distillation | 1 |
| 1.2 Propylene/Propane fractionator | 2 |
| 1.3 Objective of the thesis | 6 |
| | |
| Chapter 2: Mathematical Model Development | 7-16 |
| 2.2 MESH equations for analytical modeling | 8 |
| 2.3 General strategy of mathematical solution | 11 |
| 2.4 Synthesis of equilibrium stage process | 12 |
| 2.5 Inside-Out Method | 17 |
| | |
| Chapter 3: Introduction to Simulation | 20-31 |
| 3.1 About Simulation package ASPEN HYSYS | 21 |
| 3.2 Selecting thermodynamic models for process simulation | 22 |
| 3.3 Selecting phase Equilibria method | 23 |
| 3.4 Procedure for simulation | 30 |
| | |
| Chapter 4: Simulation results | 32-41 |
| 4.1 Plant data | 32 |
| 4.2 Design case | 34 |
| 4.3 Starting the Simulation | 34 |
| 4.4 Results | 41 |

Chapter 5: Sensitivity Study

| | |
|--|--------------|
| Work book results obtained from ASPEN HYSYS | 42-48 |
| 5.1 Work book on C3 Splitter | |
| 5.2 Connections page | |
| 5.3 Solver page | |
| 5.4 Vessel dynamic specification | |
| 5.5 Datasheet of feed, PGP, CGP, Bottom | |
| 5.6 Recovery | |

Chapter 6: Closing thoughts

50-59

| | |
|--|----|
| 7.1 Results & Discussion | 50 |
| 7.2 Recent developments on C ₃ Splitter | 51 |
| 7.3 Demand/Supply of propylene | 56 |
| 7.4 Conclusion. | 60 |

| | |
|---------------------|-----------|
| Nomenclature | 61 |
|---------------------|-----------|

| | |
|-------------------|--------------|
| References | 62-63 |
|-------------------|--------------|

List of tables:

| Table No. | Description | Page. No |
|------------------|--|-----------------|
| Tab 3.1 | Simulation Packages | 20 |
| Tab 3.2 | Classification of mixtures | 24 |
| Tab 3.3 | Selection of phase equilibria method | 24 |
| Tab | EOS(Equation of State) VS ACM(Activity Coefficient models) | 27 |
| Tab | SRK(Soave-Redlich-Kwong) VS PR(Peng Robinson) Models | 29 |
| Tab 5.1 | Trays VS Packings | 43 |
| Tab 5.2 | Types of trays differentiation | 44 |

List of figures:

| Figure No. | Description | Page. No. |
|-------------------|--|------------------|
| Fig 1.1 | Typical olefins plant | 04 |
| Fig 1.2 | flowchart of Fluid catalytic cracking | 05 |
| Fig 2.1 | Distillation column with one feed, one side Stream, total condenser & partial reboiler | 16 |
| Fig 2.2 | Inside-out method Algorithm | 18 |

List of charts:

| Chart No. | Description | Page No. |
|------------------|---------------------------------------|-----------------|
| Char 3.1 | Decision making chart (Temperature)-1 | 25 |
| Char 3.2 | Decision making chart (Pressure)-2 | 26 |

List of plots:

| Plot No. | Description | Page No. |
|-----------------|---------------------------------------|-----------------|
| Plot 1 | Pressure VS tray position from top | 47 |
| Plot 2 | Temperature VS tray position from top | 47 |
| Plot 3 | Column Properties VS tray position | 48 |
| Plot 4 | Flow VS tray position from top | 48 |
| Plot 5 | K-value VS tray position from top | 49 |
| Plot 6 | Composition VS tray position from top | 49 |

Chapter: 1

INTRODUCTION

Separations are “big business” in chemical processing. It has been variously estimated that the capital investment in separation equipment is 40-50 % of the total for a conventional fluid processing unit. Of the total energy consumption of an average unit, the separation steps accounts for about 70%. And of the separation consumption, the distillation method accounts for about 95%. In general, initial design of distillation tower involves specifying the separation of a feed of known composition and temperature. Constraints require a minimum acceptable purity of the overhead and/or bottoms product. The desired separation can be achieved with relatively low energy requirements by using a large number of trays, thus incurring large capital costs with the reflux ratio at its minimum value. On the other hand, by increasing the reflux ratio, the overhead composition specification can be met by a fewer number of trays but with higher energy costs. In particular, the optimization of reflux ratio is attractive for distillation columns that operate with:

1. High reflux ratio.
2. high differential product values between overhead and bottom
3. high utility costs
4. low relative volatility
5. feed light key far from 50%

In this project we explore a distillation column used in Petrochemical Complex: called Propylene splitter, an existing tower in a Naptha Cracking Process Plant.

1.1 Distillation:

Distillation is defined as a process in which a liquid or vapor mixture of two or more substances is separated into its component fractions of desired purity, by the application and removal of heat. It is also one of the most energy intensive operations. Hence, optimization of distillation column design and operation should get high priority.

The difference between liquid and vapor compositions is the basis for distillation operations. Relative volatility is a measure of the differences in volatility between two components, and hence their boiling points. It indicates how easy or difficult a particular separation will be. The relative volatility of component 'i' with respect to component 'j' is defined as

$$\alpha_{i,j} = \frac{y_i/x_i}{y_j/x_j}$$

Numerous distillation heuristics (rules of thumb) for quick optimization have emerged over the years[1]. For instance, heuristics on optimal reflux ratio as a certain multiple of the minimum reflux ratio have been widely used as quick tools to estimate optimum reflux ratio.

However, changes over time in the relative cost of equipment and energy (which affects operating cost) can affect the validity of such rules of thumb. Meanwhile, it has now become more feasible to assess their validity, as today's availability of commercial simulators and high-speed computers allows rigorous and thus more accurate distillation calculations be carried out with relative ease.

Distillation columns present challenging:

- design problems
- Energy integration Problems
- Control problems

Rigorous modeling and simulation has proven to be insightful and productive process.

1.2 Propylene/Propane Fractionator (C₃ Splitter):

Distillation columns that separate close – boiling components have the dynamic feature of very large time constants. There are large no. of distillation columns that separate very close boiling materials. These fractionator applications include the separation of number important isomers, some alcohols, mixed butylenes and

ethylbenzene/styrene. Probably the most common and commercially most important example is the separation of propylene and propane.

Columns that make these difficult separations are characterized by very high reflux ratios (greater than 10), large no. of trays (more than 100), and very long time constants (2-10h or more). The systems are usually binary. Temperature gradients are very small, so direct composition measurements are usually required.

Propylene production is projected to come from a number of sources, both refinery and Petrochemical-complex based. On the refinery side, propylene production is from FCC units and on the petrochemical side; there are more alternatives but mainly from steam cracker. (Refer Fig:1 & 2)

Indian Petrochemicals Corporation Limited (Vadodara Complex, India) has operated a propylene unit at the back end of the olefins plant (Naphtha cracker) since from 1972. The purpose of the unit is to separate a C₃ stream into a top product containing 99% pure polymer grade propylene, side stream containing 94% pure chemical grade propylene and a bottom product containing 98% of propane. The separation has achieved conventionally by low temperature and/or high pressure distillation. This makes the propylene/propane one of the most energy expensive separations because of the low relative volatility.

Propylene is the most important building block in any petrochemical industry. Demand for propylene is ever increasing and mixtures including olefins produced in the petroleum refining process and petrochemical complex are often used as fuel. Therefore, the recovery of olefins in this stream would be a substantial conservation of resources

A strong financial incentive exists for tight control of top product purity given the high premium for polymer grade propylene. Propylene give away in the bottom product is to be minimized given \$230 per tonne price differential between propylene and propane.

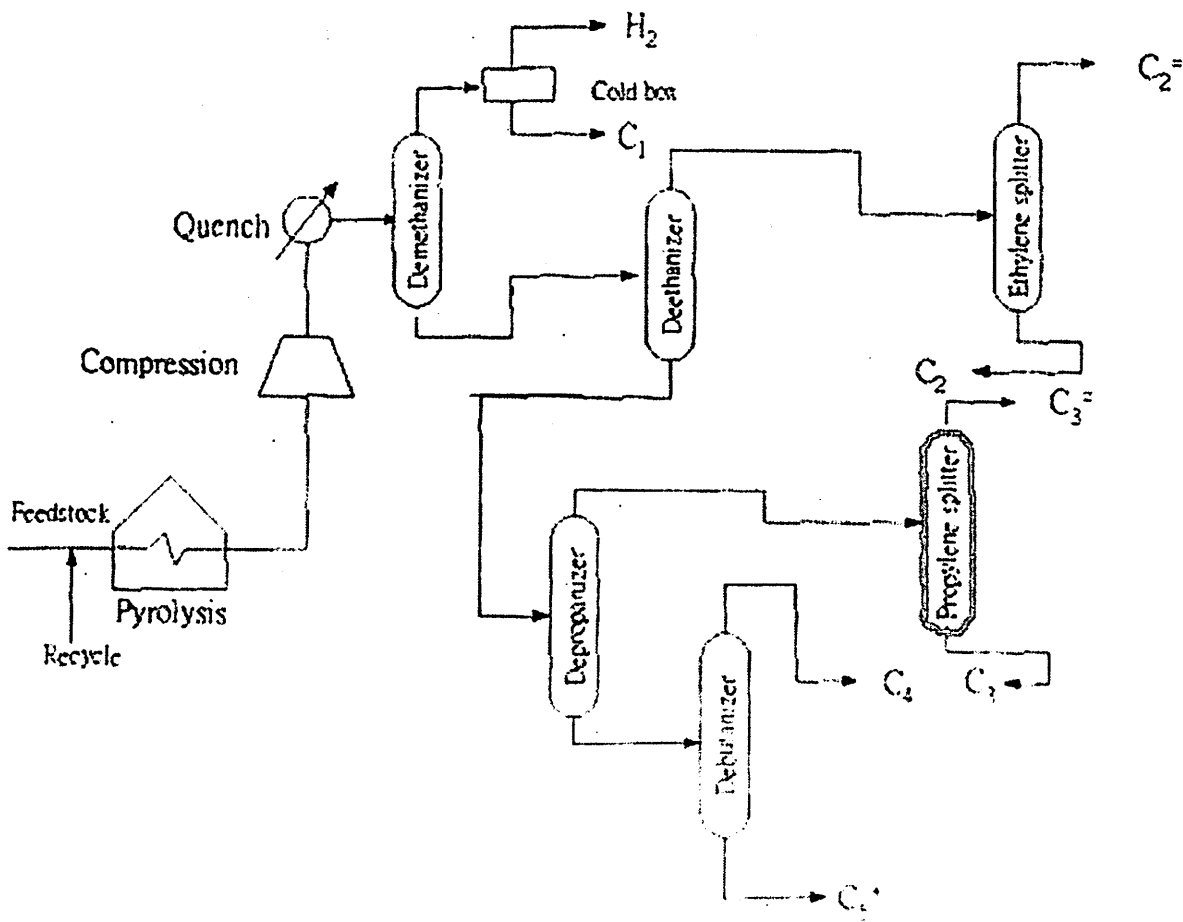


Figure 1. Typical Olefins Plant

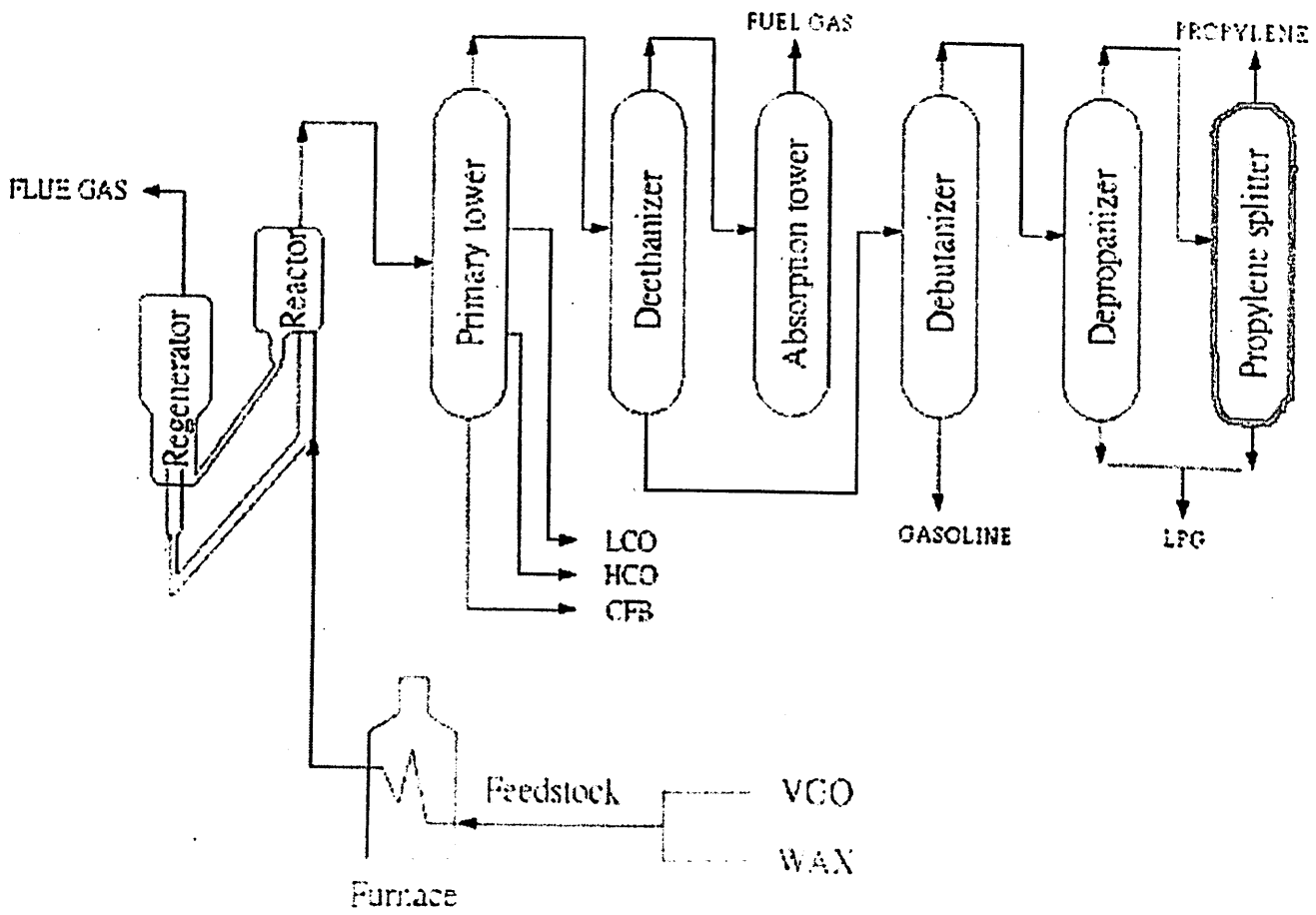


Figure 2. Flow Chart of Fluid Catalytic Cracking

1.3 Objective of the Thesis:

The separation of olefin/paraffin is quite complex because the characteristics of the molecules are similar. Large efforts are being done to cryogenic distillation for olefin/paraffin separation. Experimental steady state and dynamic plant data used to obtain steady state models. Then computer simulation studies were performed for a number of conventional and non conventional structures.

The main objective of thesis work was modeling of C₃ splitter and simulate it by using ASPEN HYSYS.

The lighter component (key element) propylene is more valuable than propane. The overhead stream has to be at least more than 97% of pure propylene and bottom product should not contain more than 5% of propylene. Based on the two component system we have to find optimum reflux ratio and minimum number of stages to accomplish the separation efficiently.

In C₃ splitter which I collected plant data from IPCL plant, it has achieved its purity of propylene at the top, but where as at the bottom the valuable product propylene was loosing 50% (considering economics) along with propane which is used as fuel. The main objectives were checking the plant data and do the modeling with necessary variables and simulate it by using ASPEN HYSYS.

Chapter: 2 MATHEMATICAL MODEL DEVELOPMENT

Introduction:

Mathematical models used for chemical process simulation and design are increasingly large due to the inclusion of many equipment details and of realistic descriptions of the physico-chemical behavior of the materials processed. Expressions for the physico-chemical properties of materials, such as fugacity or activity coefficients, are often long and intricate, and various tests are needed before assuming that a computational implementation is correct.

Before 1950s, column calculations were performed by hand. Although rigorous calculation procedures were available, they were difficult to apply for all but very small columns[5]. Short cut methods were therefore the primary design tool. Rigorous procedures were only used for small columns or for final design checks. Inaccuracies and uncertainties in the short cut procedures were usually accommodated by over design.

The introduction of computers has entirely revised the design procedure. Rigorous calculations, once taking several days, sometimes weeks, for even a relatively simple column, can now be performed quickly using a computer. In modern distillation practice, rigorous methods are primary design tool.

With the superior accuracy and capabilities of modern rigorous methods, a column should not be designed without them. A short cut calculation is inferior in accuracy, and in some cases may give misleading results. In most modern column design work, the role of shortcut calculations is restricted to eliminating the least desirable design options, providing the designer with an initial estimate for rigorous step and for trouble shooting the final design. The rigorous methods are used as the primary design and optimization tool.

The mathematical model can be developed in two ways:

1. Short cut methods(or Approximate method)
2. Rigorous computer methods

Short cut methods are commonly referred to as the *fenske-underwood-gilliland* or *FUG* method. In addition, application of the *kremser* method is extended to and illustrated for strippers and extraction. These methods are suitable only for preliminary design studies (multi stage separation, such as binary distillation) like estimation of stage and reflux requirements.

Rigorous methods are used for final design of multistage equipment for conducting multi component separations requires determination of temperature, pressure, stream flow rates, stream compositions, and heat transfer rates at each stage. This determination is made by solving material balance (M), enthalpy balance (H), and equilibrium relations (E) at each stage. These relations are nonlinear algebraic equations that interact strongly. Solution procedures are relatively difficult and tedious. A wide variety of iterative solution procedures for solving nonlinear algebraic equations were available. Choosing the best possible method is important. Once the procedures are programmed for high speed digital computer (Simulation), solutions are achieved fairly rapidly and almost routinely.

MESH equations for analytical modeling:

The basic equations below fully describe a distillation column. They must be satisfied in any solution technique. These equations define the overall column total material balances, energy balances and product compositions. Internal to the column, they describe equilibrium conditions, internal (stage-to-stage) component and total material balances, and enthalpy balances. The independent variables of a column are the product rates and composition, internal vapour and liquid rates and compositions, and stage temperatures. Equilibrium constants, K-values, and mixture enthalpies are dependent variables. Each stage is assumed to be at equilibrium (a theoretical stage), though an efficiency can be applied in the equation.[5]

The rigorous methods thus convert a column to a group of variables and equations.

The MESH variables are often referred to as state variables.

Here i = No. of stages

j = No. of components

M equations-material balance for each component(C equations for each stage):

The summation equation or composition constraint states that the sum of the mole fractions on each stage is equal to unity.

$$M_{i,j} = L_j x_{i,j-1} + V_{j+1} y_{i,j+1} + F_{j,z} z_{i,j} - (L_j + U_j) x_{i,j} - (V_j + W_j) y_{i,j} = 0$$

$$i = 1, 2, \dots, N (= 182)$$

$$j = 1, \dots, C (= 2)$$

N = total no. of equilibrium stages

C = total no. of components in the feed.

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 equilibria ratio.

$$i = 1, 2, \dots, N (= 182)$$

$$j = 1, \dots, C (= 2)$$

N = total no. of equilibrium stages

C = total no. of components in the feed.

S equations – mole fraction summations(one for each stage)

$$(S_y)_j = \sum y_{i,j} - 1.0 = 0$$

$$(S_x)_j = \sum x_{i,j} - 1.0 = 0$$

H equations – energy balance(one for each stage)

$$H_j = L_{j-1}h_{j-1} + V_{j+1}hv_{j+1} + F_jhF_j - (L_j + U_j)hL_j - (V_j + W_j)hv_j - Q_j = 0$$

Where kinetic and potential energy changes are ignored.

$$i = 1, 2, \dots, N (= 182)$$

$$j = 1, \dots, C (= 2)$$

N = total no. of equilibrium stages

C = total no. of components in the feed.

The bubble point and Dew point equations:

The equilibrium equation and composition constraint are combined to get the bubble point equation,

$$\sum y_i = 1$$

And the dew point equation:

$$\sum x_i = 1$$

The bubble point and dew point equations are used in some of the solution methods to help determine the stage temperature.

Tray efficiencies:

To characterize the deviation from ideality, stage efficiencies are often used. Most computer simulations work with ideal stages. Once the no. of ideal stages is established, the number of actual trays is calculated using stage efficiencies. Commonly, a Murphree vapour efficiency used for each component, given as

$$E_{MV} = \frac{y_{ij} - y_{ij+1}}{y^*_{ij} - y_{ij+1}}$$

Where y^*_{ij} = vapour composition would be if the vapour were equilibrium with the actual liquid on the stage and y_{ij} , and y_{ij-1} an actual vapour compositions.

2.2 General strategy of Mathematical Solution:

- **Pre computer methods:**

The Thiele-Geddes and Lewis-Matheson methods are rigorous methods referred to as stage-to-stage methods. Both preceded the computer and are suitable manual calculations.[5]

- **Classification of methods:**

1. The bubble point method(BP)
2. The sum rates method(SR)
3. The 2N Newton methods
4. The simultaneous correction method(SR)
5. Inside-out methods
6. Relaxation methods
7. Homotopy methods
8. Non equilibrium models

The Thiele-Geddes method, where the no. of equilibrium stages above and below the feed, the reflux ratio, and the distillate flow rate are specified, and the stage temperature and interstage vapour (or liquid) flow rates are the iteration (tear) variables. However, it was found to be numerically unstable when attempts were made to program it for digital computer.

The Lewis Matheson method is also an equation tearing procedure. It was formulated to determine stage requirements for specifications of the separation of two key components, a reflux ratio and a feed stage location criterion. This method was widely used for hand calculations, but it also proved often to be numerically unstable when implemented on a digital computer.

Bubble point (BP) method is restricted to distillation problems, for separations where the feed(s) contains only components of similar volatility (narrow boiling range).

Sum rate (SR) method is generally restricted to stripping, absorption, extraction problems, for a feed(s) containing components of widely different volatility (wide boiling case) or solubility.

The simultaneous correction (SC) and inside-out methods are designed to solve any type of column configuration for any type of feed mixture. Because of its computational efficiency, the inside-out method is often the method of choice; however, it may fail to converge when highly nonideal liquid mixture are involved, in which case the slower SC method should be tried. Both methods permit considerable flexibility in specifications.

Relaxation and homotopy methods can be tried, when both the SC and inside-out methods fail.

2.3 Synthesis of equilibrium stage process:

The first step in the analysis of any system is to count the total number of variables N_v . The number N_v is analogous to the number of unknowns in a system of simultaneous algebraic equations. The second step is to count all the restricting conditions or relationships existing in the system. The number of such restrictions will be denoted as N_c . These restrictions are analogous to the independent equations which can be written in an algebraic system. If the number of equations are equals the number of unknowns, a unique solution is possible. Likewise, if the number of restrictions N_c existing in a system equals the total number of variables N_v , then the system is completely defined. Such an equality does not often exist in the typical design problem. Then, just as in the case of an algebraic system, the designer must arbitrarily specify certain variables. The number which he can specify is referred to as the degrees of freedom in the system and can be calculated by the following equation.

$$N_i = N_v - N_c$$

Where N_v = total no. of variables

N_c = total no. of restrictions (or constraints or equations)

N_i = degrees of freedom (or called as design variables, since these are the variables which the designer must specify to define the design problem completely).

Propylene/Propane fractionator contains:

Column with one feed stream, one side stream, reflux ratio, total condenser, partial reboiler

Stream divider: A divider (reflux) simply splits a stream into two or more product streams.[6]

$$N_v = 3(C+2) - 1 = 3C + 7$$

$$N_c = 2C + 2$$

$$N_i = N_v - N_c = C + 5$$

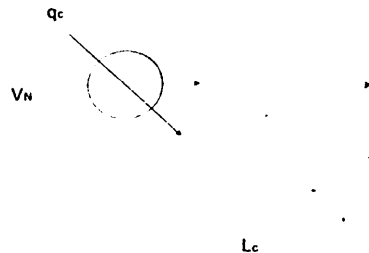
Each material stream contributes $C+2$ variables.

Total condenser: The condenser is described as total when all the vapour feed is condensed to a liquid.

$$N_v = 2(C+2) + 1$$

$$N_c = C + 1$$

$$N_i = C + 4$$

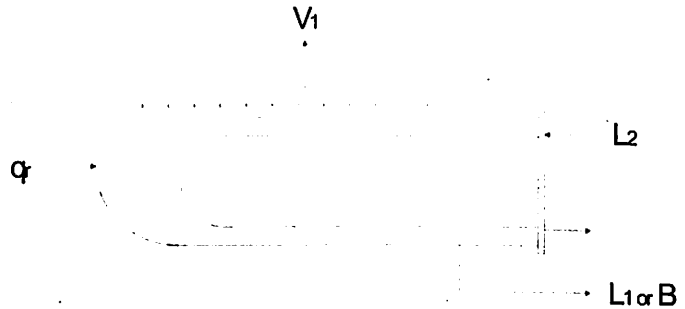


Partial Reboiler: If the reboiler causes only part of the entering stream to change phase, it is termed a partial reboiler. Partial reboilers are always assumed to be equilibrium stages in so far as the separations are always assumed is concerned.

$$N_v = 3(C+2) + 1$$

$$N_c = 2C+3$$

$$N_i = C+4$$

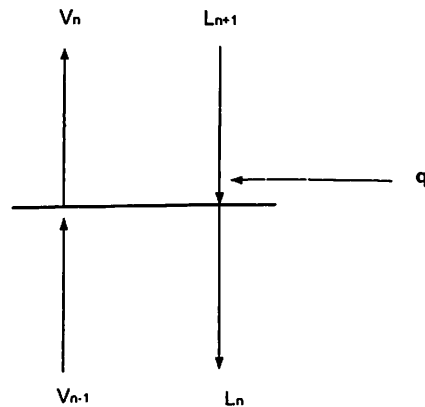


Simple Equilibrium Stage: A schematic representation of a simple equilibrium stage (no fresh feed or side stream). Four material streams and one heat stream involved.

$$N_v = 4(C+2) + 1$$

$$N_c = 2C+3$$

$$N_i = 2C+6$$

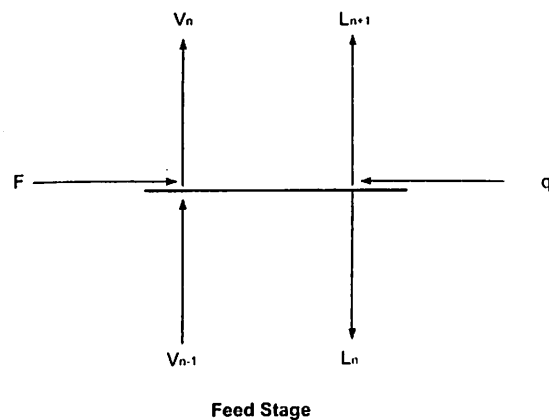


Feed stage: A feed stage differs from a simple equilibrium stage in that a fifth material stream F is involved.

$$N_v = 5(C+2) + 1$$

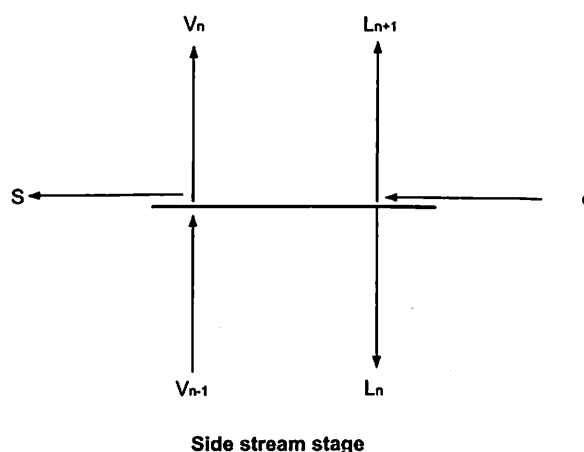
$$N_c = 2C+3$$

$$N_i = 3C+8$$



Side Stream Stage: A side stream stage is an intermediate stage in a series of simple equilibrium stages from which a product stream is withdrawn. The side stream may be returned to another stage after cooling or heating, but this is immaterial at this stage of the analysis. [6]

Since five material streams and one heat stream are involved, the total no. of variables is same as for a feed stage, namely $5C+11$. The no. of restricting relationships N_c is not the same as for feed stage. The stream S must be identical in composition with either V_n or L_n and also have the same temperature and pressure as L_n and V_n . Therefore, $C+1$ identities or restricting relationships must exist between S and L_n or V_n .



$$N_v = 5(C+2) + 1$$

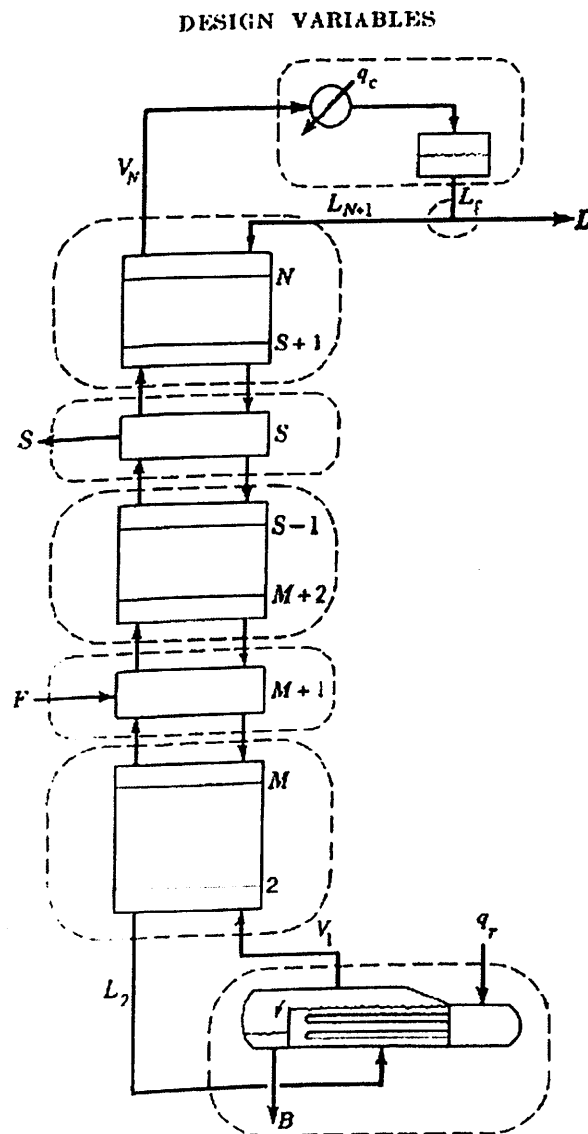
$$N_c = (C+1) + (2C+3)$$

$$N_i = 2C+7$$

This number exceeds that for a simple equilibrium stage by one, and this additional degree of freedom would probably be used to specify the rate of S . The composition, temperature, and pressure of S are fixed by the specifications usually made for the equilibrium stage.

Combination of Elements to form units:

Distillation column with one feed, one side stream, total condenser, and partial reboiler: (Propylene/Propane fractionator) (fig:2.1)



| <i>Element</i> | $N_v = \sum N_i$ |
|--|-------------------------------|
| Total condenser | C+4 |
| Divider (reflux) | C+5 |
| (N-S) simple equilibrium stages | $2C+2(N-S) +5$ |
| Side stream | $2C+7$ |
| (S-1)- (M+1) simple equilibrium stages | $2C+2(S-M-2) +5$ |
| Feed stage | $3C+8$ |
| (M-1) simple equilibrium stages | $2C+2(M-1)+5$ |
| Partial reboiler | <u>C+4</u> |
| | <u>$14C+2N+37$</u> |

The addition of side stream to the unit increases the number of elements. Thirteen inner streams give an

$$N_c = 13(C+2)$$

Then, $N_i = C+2N+11$

The addition of side stream has increased the degrees of freedom by two. These two degrees of freedom could be used to specify the rate of S and the number of stages between the side stream and feed stages.

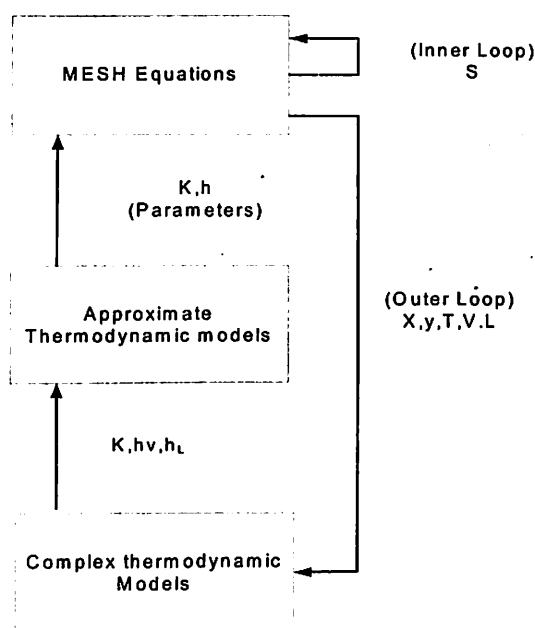
2.4 Inside-out Method:

In bubble point method(BP), Sum rate(SR) method and Simultaneous correction(SC) method, a large percentage of the computational effort is expended in calculating K-values, vapor-phase enthalpies and liquid phase enthalpies, particularly when rigorous thermodynamic property models(e.g., SRK, PR, Wilson, NRTL, UNIQUAC) are utilized.[7]

Boston and Sullivan presented an algorithm designed to significantly reduce the time spent in computing thermodynamic properties when designing steady state, multi component separation operations.

As shown in figure 2.2 , two sets of thermodynamic property models are employed:

1. A simple approximate empirical set used less often in converge inner loop calculations.
2. The rigorous complex set used less often in the outer loop.



The MESH equations are always solved in inner loop with the approximate set. The parameters in the empirical equations for the approximate set are updated in the outer loop by the rigorous equations, but only at infrequent intervals. A distinguishing feature of the Boston-Sullivan method is these inner and outer loops; hence the name *inside-out* for this class of methods. It is also called as *two-tier* method.

The inside-out method in 1974, the development and application was restricted to hydrocarbon distillation (moderately non ideal systems), but with multiple feeds, side streams and intermediate heat exchangers. For these applications, the inside-out was shown rapid and robust. These extensions permit the inside-out method to be applied to almost any type of steady state multi component, multi stage vapour liquid separation operation.

The inside-out method takes advantage of the following characteristics of the iterative calculations:

1. Component relative volatility varies much less than component K-values.
2. Enthalpy of vaporization varies less than phase enthalpies.
3. Component stripping factors combine effects of temperature and liquid and vapor flows at each stage.

The inner loop of the inside-out method uses relative volatility, energy and stripping factors to improve stability and reduce computing time.

The main assumptions adopted for the model development are as follows:

1. Liquid on the tray was perfectly mixed and incompressible.
2. The molar vapor holdup was negligible compared to the molar liquid holdup.
3. The liquid and vapor leaving each plate were in thermal equilibrium (same temperature) but not in phase equilibrium (Murphree vapor-phase efficiency = 100%).
4. Vapor-liquid equilibrium (VLE) was calculated using the SRK (Soave-Redlich-Kwong) thermodynamic model.
5. Equi molal overflow.
6. Heat losses up the column and temperature changes from tray to tray (sensible heat effects) are assumed negligible.

These assumptions mean that the vapor and liquid rates through the stripping and rectifying sections will be constant under steady state conditions.

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.[12]

Table: 3.1 Simulation packages

| Acronym | Type | Internet Address |
|-------------|-----------------------|------------------|
| ASPEN PLUS | Steady state | Aspentech.com |
| DESIGN II | Steady state | Winsim.com |
| ASPEN HYSYS | Steady state | Hyprotech.com |
| PRO II | Steady state | Simsci.com |
| DYNSIM | Dynamic | |
| CHEMCAD | Steady state | Chemstations.net |
| UNISIM | Steady state, Dynamic | Honeywell.com |

In this case (Propylene/Propane Fractionators), HYSYS from Aspentech 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. Heat integration, process recycles and minimum hold-ups are typical design features. Whilst such design optimizes steady state operation, they present particular challenges to plant control and operational engineers.

3.1 About Simulation Package: ASPEN HYSYS

Aspen HYSYS is an integrated steady-state process simulation package application that brings new levels of productivity and profitability throughout the plant lifecycle.[9] Aspen HYSYS helps engineers to create simulation models for:

- Plant design
- Performance monitoring
- Troubleshooting
- Operational improvement
- Business planning
- Asset management

- **Comprehensive thermodynamics foundation.**

Aspen HYSYS ensures accurate calculation of physical properties, transport properties, and phase behavior; and contains an extensive component database with the ability to add user components.

- **Clear and concise graphics.** Aspen HYSYS provides PFDs that offer a graphical representation of the process flow sheet, productivity features, and graphics that depict comprehensive unit operations.

- **Integration with other AspenTech and third party Applications.** Aspen HYSYS interfaces easily with applications such as Microsoft Excel and Visual Basic, and features Active X compliance.

The simulation software Aspen HYSYS is a desktop package for both steady state and dynamic simulation. It has long been recognized that engineering effort in simulation activities can be minimized by reusing models. However, the full potential of simulation for the design and tuning of control strategies has not been fully exploited to date, for numerous reasons, including lack of awareness of the technology and maintenance costs.

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.[9]

Simulation generally differs from hand calculations in two ways: (1) the simulator allows use of more sophisticated models without significantly expending more of the engineer's time and (2) simulations in chemical engineering typically involve VLE (vapor-liquid equilibrium) where the ideal gas EOS (equation of state) is inaccurate. Productivity is rarely diminished by selecting rigorous thermodynamic models as

Compared to models that make for easy calculations, and so, criteria for selecting thermodynamic models during simulation are based primarily on accuracy and not the optimal combination of accuracy and effort. However, acquiring accurate binary interaction coefficients or data still fall within the realm of increasing accuracy at the expense of increased effort.

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.

Selection of vapor pressure models, pure component fugacity models, or other methods such as interpolation of available data are typically performed automatically by simulation packages only as necessary and without operator interaction.

3.3 Selection of Phase Equilibrium method:

The choice of the best method for deducing vapour-liquid and liquid-liquid equilibria for a given system will depend on three factors:[12]

1. The composition of the mixture (the class of the system)
2. The operating pressure(low, medium or high)
3. The experimental data available.

Table: 3.2 classification of mixtures

| | Class | Principle interactions | Examples |
|-----|-----------------------------|------------------------|---|
| I | Simple molecules | Dispersion forces | H ₂ , N ₂ , CH ₄ |
| II | Complex non polar molecules | Dispersion forces | CCL ₄ , I C ₅ H ₁₀ |
| III | Polarisable | Induction dipole | CO ₂ , C ₆ H ₆ |
| I V | Polar molecules | Dipole moment | Dimethyl formaldehyde, chloroethane |
| V | Hydrogen bonding | Hydrogen bonds | Alcohols, water |

Table: 3.3 selection of phase equilibria method

| Class of mixture | Low <3 bar | | Pressure moderate <15 bar | | High >15 bar | |
|-----------------------------------|------------|----------|---------------------------|----------|--------------|----------|
| | F_l | f_v | F_l | F_v | F_l | F_v |
| I, II, III (none supercritical) | ES | I | ES | ES | ES | ES and K |
| I, II, III (supercritical) | ES | I | ES | ES | ES | ES and K |
| I, II, III, IV, V (vapor-liquid) | ACT | I | ACT | ES | ES | ES and K |
| I, II, III, IV, V (liquid-liquid) | ACT | I | ACT | ES | ES | ES |
| Hydrocarbons & water | ES | ES and K | ES | ES and K | ES | ES and K |

I = ideal, vapor fugacity = partial pressure

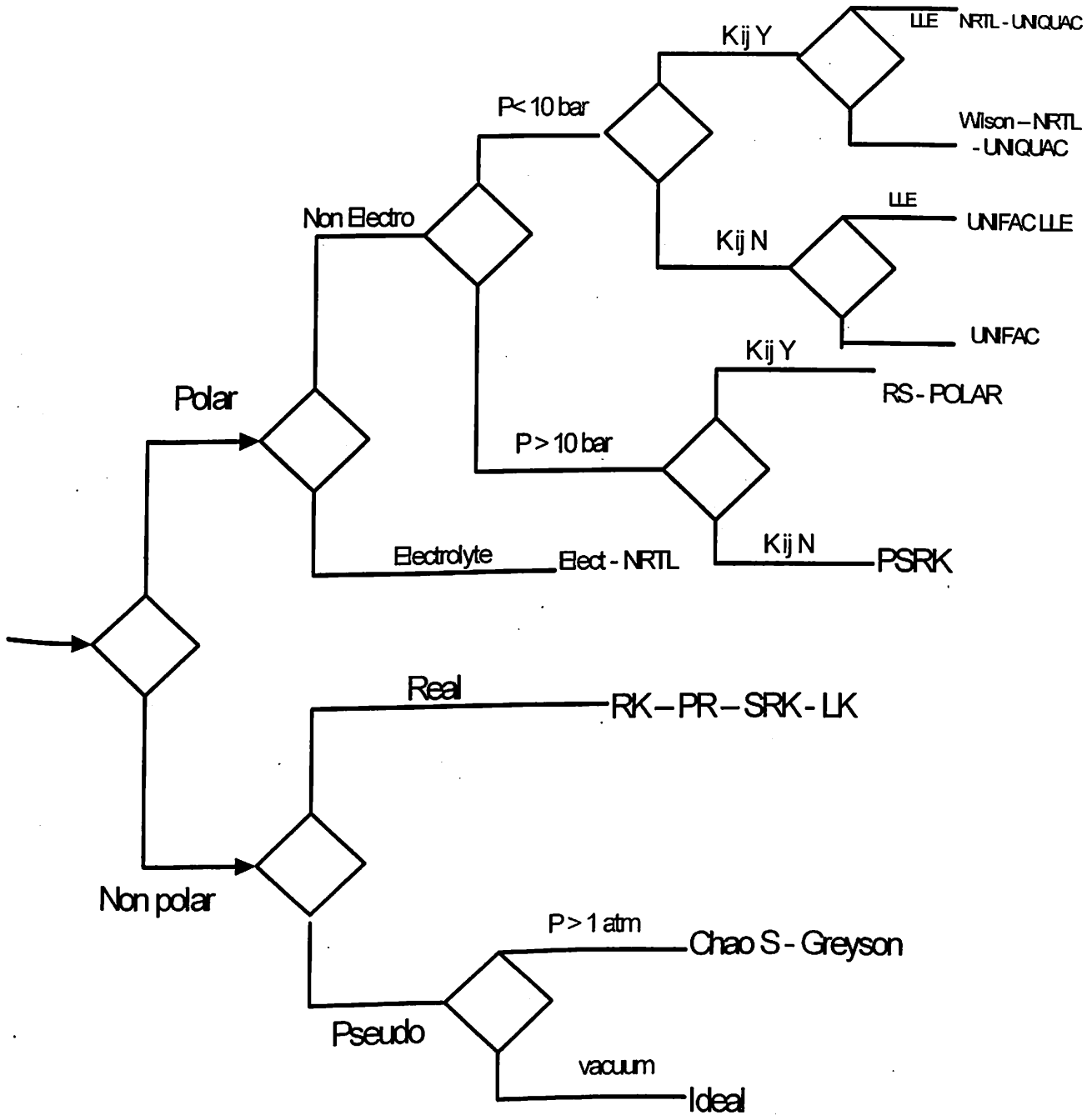
ES = approximate equation of state

K = equilibrium constant (K factor) derived from experimental data.

ACT = liquid phase activity coefficient

Decision making charts:

WITH PRESSURE-1:



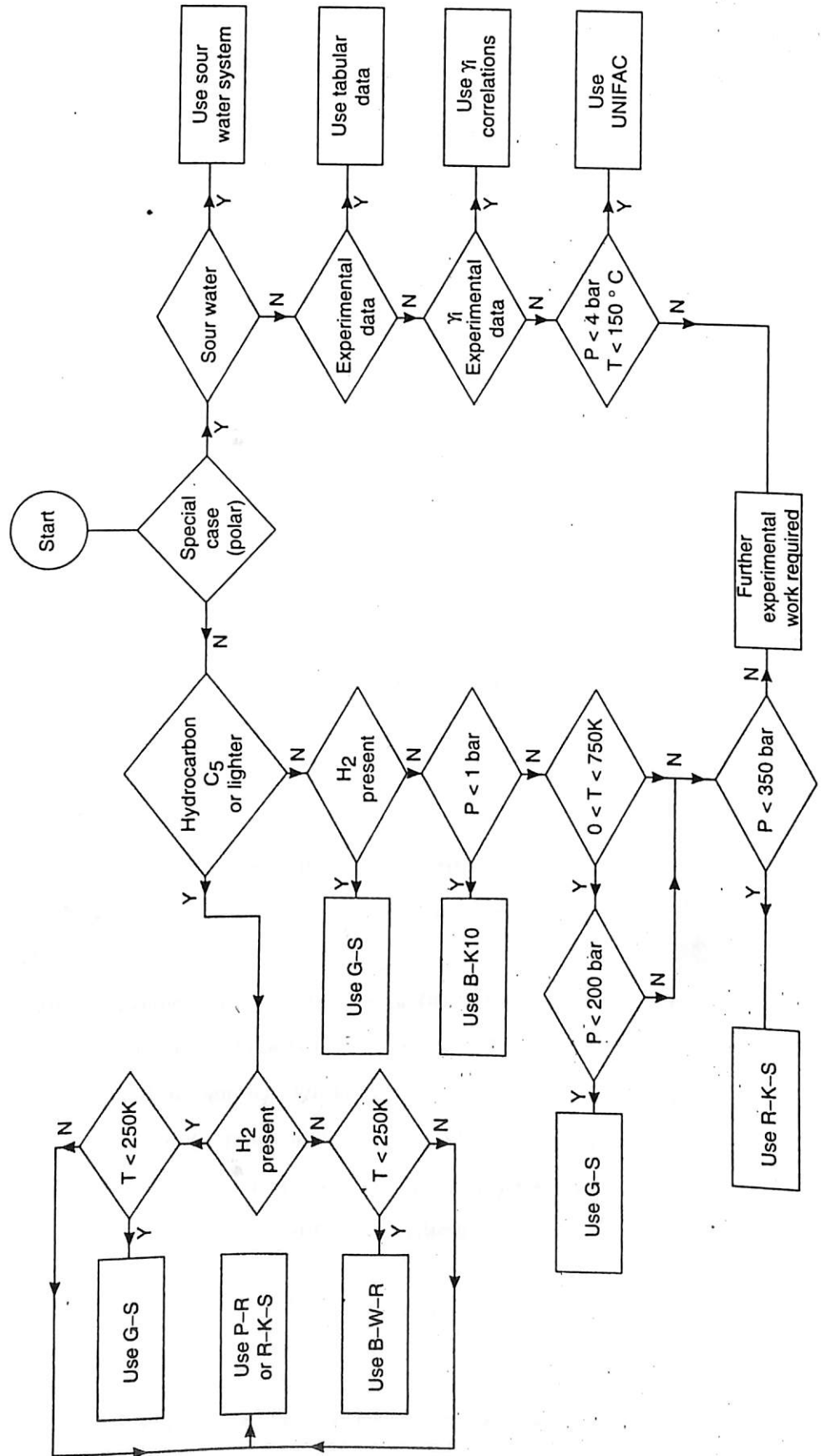


Figure 8.4. Flow chart for the selection of phase equilibria method

Equation of state VS Activity coefficient Models:

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. [13]
- ✓ 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 CO₂ 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.

Activity co-efficient models:

- ✓ Unlike EOS models, Gibbs Excess/Activity Coefficient models calculate infinite dilution and mixture properties for the liquid phase only, and cannot calculate pure properties or vapor phase properties.
- ✓ When a Gibbs Excess/Activity Coefficient model is selected, liquid properties are calculated using the specified model, and vapor phase properties are calculated using Ideal Gas (IG), Peng Robinson (PR), or Soave-Redlich-Kwong (SRK).
- ✓ For low pressure (70 Pisa or less), Ideal Gas should be suitable for predicting vapor phase properties. For higher pressures, SRK or PR should be used to calculate vapor phase properties because they account for vapor phase imperfections at higher pressures.
- ✓ Two types of activity coefficients models: Electrolytic and Molecular Gibbs Excess/Activity Coefficient models.

Molecular Gibbs Excess/Activity Coefficient models:

- ✓ These models are applicable to binary and multi component systems and are intended to be used in chemical industry type applications.
- ✓ Gas Processing applications should instead use an EOS model for general properties and an Electrolytic Gibbs Excess/Activity Coefficient model for amine treating of hydrocarbons.
- ✓ Available Molecular Gibbs Excess/Activity Coefficient models are:

- Margules
 - NRTL
 - Wilson
 - UNIFAC LLE
 - UNIFAC VLE
 - UNIQUAC
 - Van Laar
 - Wilson
-
-

Electrolytic Gibbs Excess/Activity Coefficient models:

- ✓ Electrolytic models are applicable for systems in which dissociation of compounds is important (e.g. amine sweetening applications and systems containing ammonia and an acid gas such as H₂S or CO₂).
- ✓ Available electrolytic activity coefficient models are:
 - Electrolytic ELR
 - Electrolytic NRTL
 - Electrolytic Kent-Eisenberg
- ✓ Systems containing glycols should not be modeled using an electrolytic package. Instead, an Equation of State model such as Peng-Robinson or SRK should be used.

Soave-Redlich-Kwong (SRK) VS Peng-Robinson (PR) EOS Models:

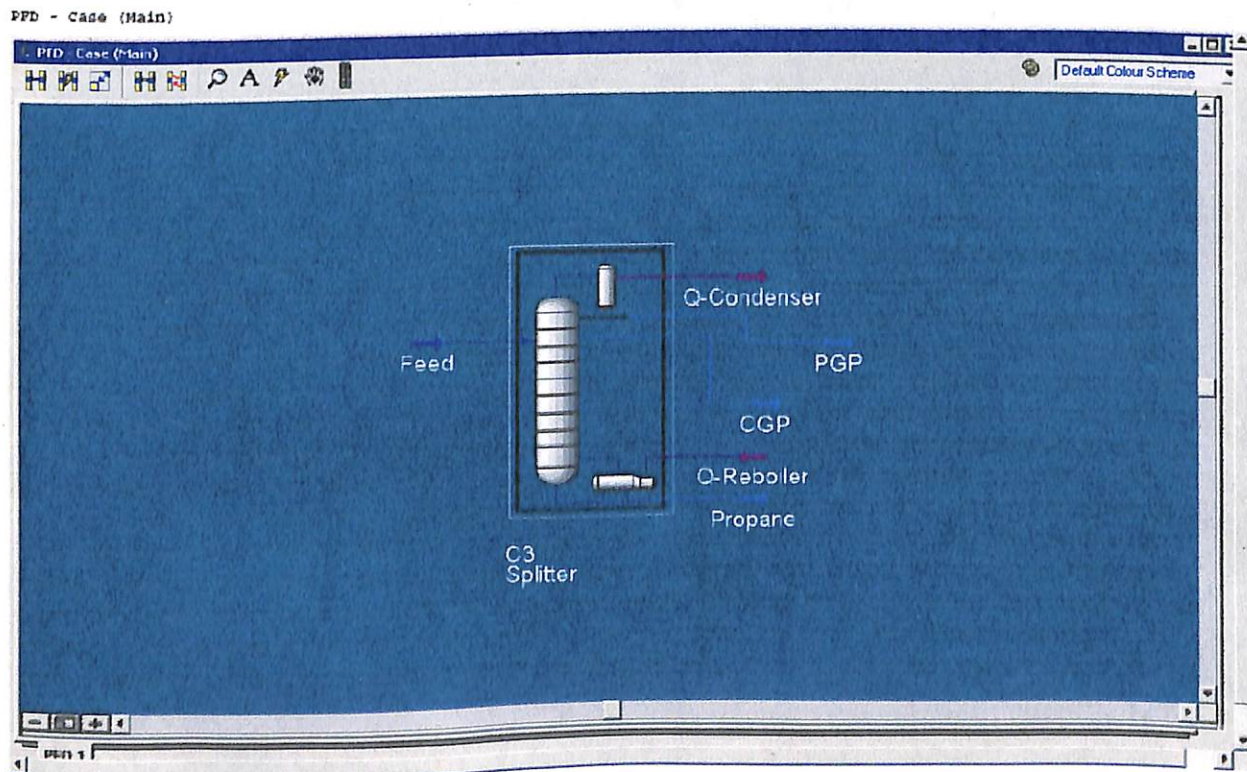
Among many equations of state proposed for predicting phase behavior (vapor-liquid equilibria) of non-polar systems, cubic equations of state Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) models are probably the most widely used in the refinery and gas processing industries because of their simplicity and accuracy. [14]

Examining the accuracy of reproducing the activity coefficients, as given in the PR and SRK equations of state produce almost identical results of all different mixing rules. Table 3 also compares the VLE predictions of the cubic equations of state. The comparisons show that there is little difference in the accuracy of the predictions with these two methods. Based on these results, it seems to indicate that both equations of state are equivalent to each other and neither one has an advantage over the other in phase equilibrium calculations as long as the alpha correlation.

The application of the PR or SRK equation of state to systems containing highly non-ideal components requires an appropriate mixing rule for the equation of state parameter a . However, their mixing rule has not become widely used because the available excess Gibbs energy parameters at low pressure cannot be used in their mixing rule.

3.4 Procedure for simulation:

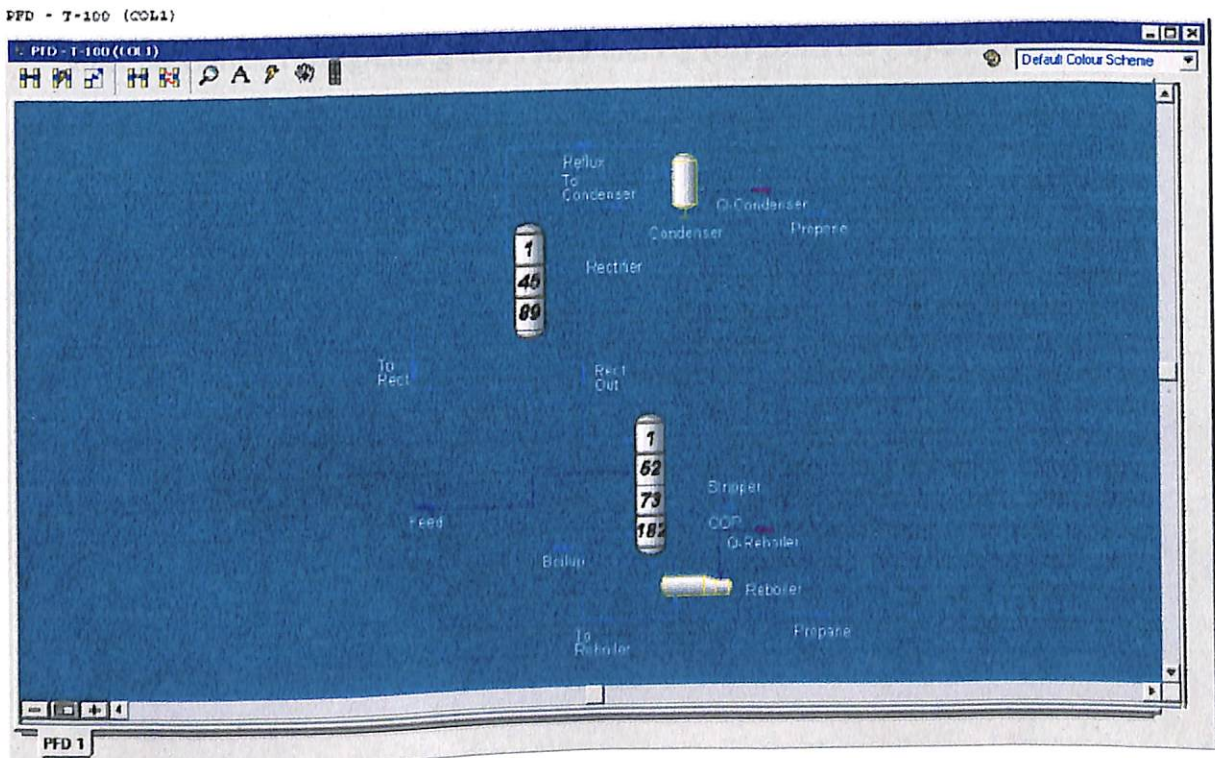
A propylene/propane splitter is generally an easy column to converge. However, the critical factor in producing good results is not the ease of solution, but rather the accurate prediction of the relative volatility of the two key components. Special consideration was given to these components, along with others, in developing the binary interaction coefficients for the Peng Robinson and Soave Redlich Kwong Equations of state to ensure that these methods correctly model this system.[9]



These splitters have many stages, and are often built as two separate columns. This simulation will contain two columns, a stripper and a rectifier. The stripper is operated as a reboiled absorber and contains 94 theoretical stages. The rectifier is refluxed absorber containing 89 theoretical stages. The stripper contains two feed streams, one is the known stream FEED, and the other is the bottom from the rectifier. Propane is recovered from the stripper bottom (95%) and propene is taken off the top of the rectifier (99%).

There are two basic steps in this process simulation.

1. **Setup:** The Soave Redlich kwong (SRK) property package will be used and the component list includes propane, propene and traces.
2. **Steady State Simulation:** The case will consist of a column divided into two tray sections: a Refluxed Absorber as a Rectifier and a Reboiled Absorber as Stripper.



4.1 Plant data:

Feed Conditions:

Feed: Propylene/propane mixture

Feed flow rate: 11.6 m³/hr

Feed condition: saturated liquid

Quantity: 12.5 TPH (or) 300 TPD

Feed plate: 102, 108, 114

Feed composition:

Propylene: 95.20%

Propane: 4.08%

Traces: 0.72 ppm

Inlet temperature of feed: 56^o C

Inlet pressure: 21.62kg/cm².g (or) 15619 mm Hg (or) 20.26 bar (or) 20.55 atm

Pressure is constant (Isobaric)

Temperature changes

Product Conditions:

Top Product: Polymer Grade Propylene (PGP) - distillate

Quantity: 10m³/hr (or) 5TPH (or) 122.14 TPD

Distillate composition:

- Propylene : 99.58%
- Propane : 0.39%
- Ethane : 9.79 ppm
- Ethylene : 0 ppm
- PD : 0
- MA : 14.07 ppm

Side stream product: Chemical Grade propylene (CGP)

Quantity: 170.61 TPD (or) 7.10 TPH (or) 15.45 m³/hr

Side stream Composition:

- Propylene : 94.87%
- Propane : 4.96%
- Ethane : 1.34 ppm
- Ethylène : 0 ppm
- PD : 0.04 %
- MA : 0.12% ppm

Bottom product conditions: Propane

Quantity: 0.89m³/hr (or) 0.34 TPH (or) 8.16 TPD

Composition:

- Methane : 0.10%
- Ethane : 0.51%
- **Propylene : 50.79%**
- Propane : 38.15 %
- PD : 4.53 %
- MA : 2.87%
- Traces : 2.45 %

Tower specifications:

Tower height: 64.95m

Tower diameter: 2.6m

Tower is made up of carbon steel and hence should not be cooled less than 0° C.

Total number of trays: 152

Tray type: Valve trays/plates

Tray spacing: 375mm (from 1 to 101 plates, from top) & 400mm (from 102 to 152 plates)

Operating conditions:

Operating pressure: 20.8 kg/cm².g
Tower pressure drop: 0.68 kg/cm².g

Operating temperature:

Base: 59.4⁰ C
Reboiler outlet: 59.4⁰ C
Overhead outlet: 49.5⁰ C
Reflux: 45.40C

Reflux:

Ratio: 18.1
Pump discharge pressure: 26kg/cm².g
Pump flow: 85648kg/hr

Quench water to reboiler:

Reboiler: Thermosphyn (2)-Horizontal
Flow: 509648 kg/hr
Temperature: 79⁰ C

Cooling water to condenser:

Flow: 10225 kg/hr
Temperature: 35⁰ C

4.2 Design case:

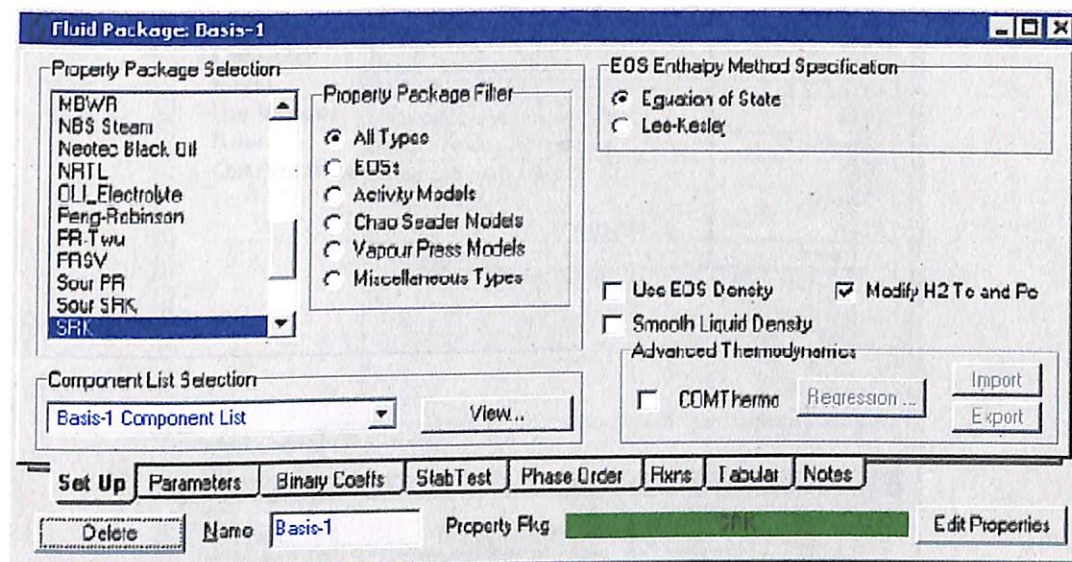
Fill the plant data results by choosing the thermodynamic package as shown below.

Steady state simulation:

The case will be setup in steady state using the custom column option. Both the rectifier and stripper columns will be built in the same column environment.[9]

4.3 Starting the simulation:

Fluid Package: Basis-1

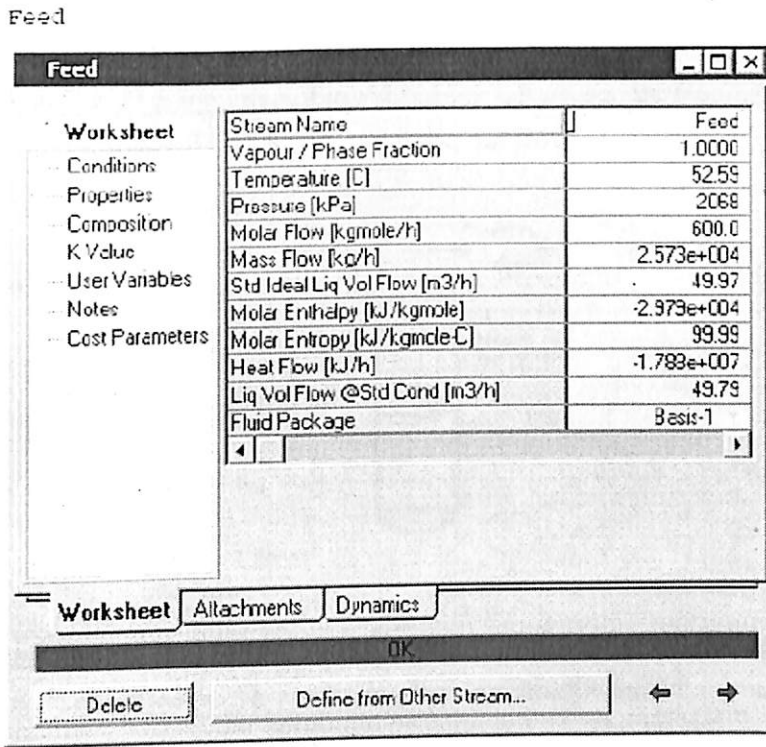


Feed stream:

The conditions and composition of the feed stream are shown below:

| Material stream [feed] | |
|---------------------------------|----------|
| In the cell... | Enter... |
| Name | Feed |
| Vapor fraction | 1.0000 |
| Pressure (Kg/cm ²) | 20 |
| Molar flow (TPD) | 300.000 |
| Comp mole fraction(propane) | 0.40 |
| Comp mole fraction(Propene) | 0.60 |

Enter this stream in the main simulation environment.



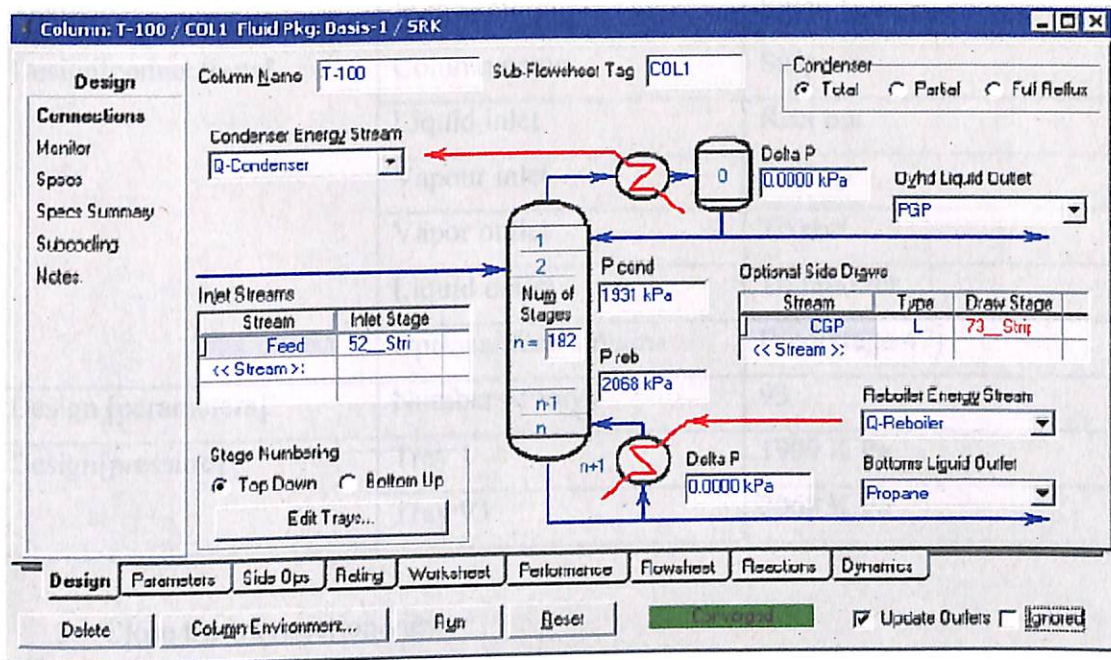
Installing the column:

The next step is to install the column.

1. Click the custom column icon on the object palette. The custom column will be used to build both columns in a single column environment.
2. Click the starting with a blank flow sheet button. Double click on the column on the PFD to open the column view.
3. Click on the flow sheet tab and open the set up page.
4. In the inlet stream group, enter the stream feed as an external feed stream, making this stream accessible to the template environment.

For this example, we need a total condenser, reboiler and two tray sections. A tray section and a condenser will be used for the refluxed absorber (rectifier), a reboiler and another tray section will be used for the reboiled absorber (stripper). The overhead product from the stripper will serve as the feed to the rectifier, and the bottom product from rectifier provides a second feed to the stripper, entering on stage 1.

Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK



Stripper (Reboiled Absorber):

The reboiled absorber is installed before the reboiler. This column has 93 ideal stages and a reboiler.

Installing the tray section:

For this column a new tray section has to be installed.

1. Double click the tray section button from the palette and it is placed on the PFD.
2. The tray section property view appears. Supply the following information on the connections and the pressures pages of the design tab.

| Tray section[stripper] | | |
|------------------------|-----------------------|----------------|
| Tab[page] | In the cell... | Enter... |
| Design[connections] | Column name | Stripper |
| | Liquid inlet | Rect out |
| | Vapour inlet | Boil up |
| | Vapor outlet | To rect |
| | Liquid outlet | To reboiler |
| | Optional feed streams | Feed(stage 47) |
| Design [parameters] | Number of trays | 93 |
| Design[pressure] | Tray 1 | 1999 K Pa |
| | Tray 93 | 2068 K Pa |

3. Close the tray section view.

Installing the Reboiler:

The reboiler for the absorber must be installed with the stripper column. Click the reboiler icon and supply the inputs shown here on the connections page of the reboiler property view.

| Reboiler [reboiler] | | |
|---------------------|-----------------|---------------|
| Tab[page] | In this cell... | Enter... |
| Design[connections] | Name | Reboiler |
| | Boil up | Boil up |
| | Inlets | To reboiler |
| | Bottom outlets | Propane |
| | Energy | Reboiler duty |

Rectifier [Refluxed Absorber]

The rectifier is installed next. This column has 89 ideal stages and a total condenser.

Installing the tray section:

Again, a new tray section must be installed for the absorber.

1. Click the tray section icon on the object palette.
2. Open the tray section property view and supply the parameters shown below.

| Tray section[Rectifier] | | |
|-------------------------|-----------------|--------------|
| Tab[page] | In the cell... | Enter... |
| Design[connections] | Column name | Rectifier |
| | Liquid inlet | Reflux |
| | Vapour inlet | To rect |
| | Vapor outlet | To condenser |
| | Liquid outlet | Rect out |
| Design [parameters] | Number of trays | 89 |
| Design[pressure] | Tray 1 | 1931 K Pa |
| | Tray 89 | 1999 K Pa |

3. Close the tray section view.

Installing the total condenser:

A total condenser is required for the column. Click the total condenser button from the palette, and supply the following parameters.

| Total condenser[condenser] | | |
|----------------------------|-----------------|----------------|
| Tab[page] | In this cell... | Enter... |
| Design[connections] | Name | Condenser |
| | Inlets | To condenser |
| | Distillate | Propene |
| | Reflux | Reflux |
| | Energy | Condenser duty |

Adding the specifications

Three specifications are given for this column.

1. flow of the rectifier distillate(propene) is
2. rectifier top stage reflux ratio is
3. composition fraction

Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK

The screenshot shows the 'Specifications' section of a distillation column simulation. The table below summarizes the data shown in the interface:

| Specification | Specified Value | Current Value | Wt Error | Active | Estimate | Current |
|---------------|-----------------|---------------|----------|-------------------------------------|-------------------------------------|-------------------------------------|
| Reflux Ratio | 16.40 | 16.4 | 0.0000 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Draw Rate | 351.1 kgmole/h | 351 | 0.0001 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Comp Fraction | 1.000e-002 | 1.000e-002 | 0.0001 | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |

Additional interface details: The 'Degrees of Freedom' is 0. The 'Update Inactive' button is visible. The bottom menu includes 'Design', 'Parameters', 'Side Ops', 'Rating', 'Worksheet', 'Performance', 'Flowsheet', 'Reactions', and 'Dynamics'. The status bar shows 'Update Outlets' checked and 'Ignored' unchecked.

Product stream:

The conditions and composition of the Product stream are shown below:

PGP

| PGP | |
|-----------------|-------------------------------|
| Worksheet | Stream Name |
| Conditions | Vapour / Phase Fraction |
| Properties | Temperature [C] |
| Composition | Pressure [kPa] |
| K Value | Molar Flow [kgmole/h] |
| User Variables | Mass Flow [kg/h] |
| Notes | Std Ideal Liq Vol Flow [m3/h] |
| Cost Parameters | Molar Enthalpy [kJ/kgmole] |
| | Molar Entropy [kJ/kgmole-C] |
| | Heat Flow [kJ/h] |
| | Liq Vol Flow @Std Cond [m3/h] |
| | Fluid Package |

| | |
|-------|------------|
| PGP | 1.0000 |
| 46.58 | 1931 |
| 351.3 | 1.478e+004 |
| 28.37 | 1.965e+004 |
| 64.98 | 6.905e+006 |
| 28.25 | Basis-1 |

Worksheet Attachments Dynamics

OK

Delete Define from Other Stream...

4.4 Results:

| Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK | | | | | |
|---|--------------------------------------|------------|------------|------------|------------|
| Worksheet | Name | Feed | Propene | Propene | CCP |
| Conditions | Molecular Weight | 42.89 | 44.08 | 42.08 | 42.10 |
| Properties | Molar Density [kgmole/m3] | 1.079 | 9.821 | 0.9943 | 10.97 |
| Composition | Mass Density [kg/m3] | 46.25 | 432.9 | 41.84 | 451.7 |
| PF Specs | Act. Volume Flow [m3/h] | 556.2 | 24.65 | 353.3 | 0.6100 |
| | Mass Enthalpy [kJ/kg] | 694.7 | -2595 | 467.2 | 154.4 |
| | Mass Entropy [kJ/kg-C] | 2.331 | 2.364 | 1.544 | 0.6959 |
| | Heat Capacity [kJ/kgmole-C] | 98.25 | 165.9 | 88.48 | 145.0 |
| | Mass Heat Capacity [kJ/kg-C] | 2.291 | 3.764 | 2.103 | 3.443 |
| | Lower Heating Value [kJ/kgmole] | 1.974e+005 | 2.044e+006 | 1.927e+006 | 1.925e+006 |
| | Mass Lower Heating Value [kJ/kg] | 4.604e+004 | 4.637e+004 | 4.580e+004 | 4.581e+004 |
| | Phase Fraction [Vol. Basis] | 1.000 | <empty> | <empty> | <empty> |
| | Phase Fraction [Mass Basis] | 1.000 | 2.122e-314 | 4.941e-324 | 2.122e-314 |
| | Partial Pressure of CO2 [kPa] | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| | Cost Based on Flow [Cost/s] | 0.0000 | 0.0000 | 0.0000 | 0.0000 |
| | Act. Gas Flow [ACT_m3/h] | <empty> | <empty> | 353.3 | <empty> |
| | Avg. Liq. Density [kgmole/m3] | 12.01 | 11.50 | 12.38 | 12.37 |
| | Specific Heat [kJ/kgmole-C] | 98.25 | 165.9 | 88.48 | 145.0 |
| | Std. Gas Flow [STD_m3/h] | 1.419e+004 | 5723 | 8305 | 158.2 |
| | Std. Ideal Liq. Mass Density [kg/m3] | 515.0 | 506.8 | 521.0 | 520.8 |
| | Act. Liq. Flow [m3/s] | 4.571e-007 | 6.845e-003 | <empty> | 1.695e-004 |

Design Parameters Side Ops Pricing Worksheet Performance Flowsheet Reactors Dynamics

Delete Column Environment... Run Reset Converged Update Outlets Ignored

Work book (Results) obtained from ASPEN HYSYS:

- Work book on C3 splitter.
- Connections page
- Solver page
- Tray sections
- Products
- Vessel dynamic specifications.
- Data sheet of FEED, PGP, CGP and BOTTOM.
- Trays VS Packings
- Vessel dynamic specifications.

| Vessel dynamic specifications | | |
|-------------------------------|------------------------|------------------------|
| Vessel | Reboiler | Condenser |
| Diameter(m) | 1.193 | 1.193 |
| Height(m) | 1.789 | 1.789 |
| Volume(m ³) | 2.000 | 2.000 |
| Liquid volume percent (%) | 50.0 | 50.0 |
| Level calculator | Horizontal cylinder | Horizontal cylinder |
| Fraction calculator | Use levels and nozzles | Use levels and nozzles |
| Vessel delta P(K pa) | 0.00 | 0.00 |
| Fixed vessel P spec(K Pa) | 2068 | 1931 |
| Fixed P Spen Active | Not active | Not active |

Table : 5.1 TRAYS VS PACKINGS [5]

| Factors favoring Trays | Factors favoring Packing |
|--|---|
| High liquid feed rate (occurs with high column pressure) | Operation under pressure |
| Large column diameter(packing poses maldistribution changes) | Low pressure drop |
| Complex columns(e.g. multiple draw offs) | Small(2-3-ft) column diameter |
| Varying feed composition | Corrosive systems(wider choices in materials of construction) |
| Easier scale up | Less prone to foaming |
| Lower overall weight | Lower liquid hold up |
| Entrained solids accommodated better | More amenable to batch operation |

Table: 5.2 Types of Trays Differentiation

| Type | Sieve trays | Valve trays | Bubble cap trays |
|------------------------------------|--|---|--|
| Capacity | High | High-very high | Moderately high |
| Efficiency | High | High | Moderately high |
| Turndown | Approx. 2 to 1. not generally suitable for variable load operation | About 4-5 to 1. Some design claim 10 to 1 or more. | Excellent, better than valve trays. Especially suitable at very low liquid rates |
| Entrainment | Moderate | Moderate | High (about 3 times higher than that of sieve trays) |
| Pressure drop | Moderate | Moderate. Older designs some what higher. Newer designs same as sieve trays | High |
| Cost | Low | Approx. 20% higher than that of sieve trays | High. About 2-3 times that sieve trays |
| Maintenance | Low | Low – moderate | Relatively high |
| Fouling tendency | Low | Low – moderate | High. Tendency to collect solids |
| Effects of corrosion | Low | Low – moderate | High |
| Availability of design information | Widely available | Proprietary, but information is readily available | Widely available |
| Main applications | Most columns if turndown is not critical | 1. most columns 2. service where turndown is a key factor | 1. very low flow conditions 2. if leakage must be minimized |
| Other | | | |



UNIVERSITY OF PETROLEUM
Calgary, Alberta
CANADA

Case Name: X:\ramkumarchandru4.hsc
Unit Set: SI
Date/Time: Wed Apr 25 11:49:21 2007

Workbook: C3 Splitter (COL1)

Material Streams

Fluid Pkg: All

| Name | Rect Out | Boilup | To Reboiler | To Rect | Propane |
|---------------------------|------------|-------------|-------------|------------|-------------|
| Vapour Fraction | 0.0000 | 1.0000 | 0.0000 | 1.0000 | 0.0000 |
| Temperature (C) | 48.20 | 58.05 | 58.04 | 48.20 | 58.05 |
| Pressure (kPa) | 1999 | 2068 | 2068 | 1999 | 2068 |
| Molar Flow (kgmole/h) | 3.860e+005 | 4.015e+005 | 4.017e+005 | 3.863e+005 | 242.0 |
| Mass Flow (kg/h) | 1.624e+007 | 1.770e+007 | 1.771e+007 | 1.626e+007 | 1.067e+004 |
| Liquid Volume Flow (m3/h) | 3.118e+004 | 3.492e+004 | 3.494e+004 | 3.121e+004 | 21.05 |
| Heat Flow (kJ/h) | 2.944e+009 | -4.122e+010 | -4.589e+010 | 7.599e+009 | -2.769e+007 |

| Name | To Condenser | Reflux | Propene | Feed | CGP |
|---------------------------|--------------|------------|------------|-------------|------------|
| Vapour Fraction | 1.0000 | 0.0000 | 0.0000 | 1.0000 | 0.0000 |
| Temperature (C) | 46.59 | 46.59 | 46.59 | 52.59 | 48.88 |
| Pressure (kPa) | 1931 | 1931 | 1931 | 2068 | 2027 |
| Molar Flow (kgmole/h) | 3.803e+005 | 3.800e+005 | 351.3 | 600.0 | 6.690 |
| Mass Flow (kg/h) | 1.600e+007 | 1.599e+007 | 1.478e+004 | 2.573e+004 | 281.6 |
| Liquid Volume Flow (m3/h) | 3.072e+004 | 3.069e+004 | 28.37 | 49.97 | 0.5408 |
| Heat Flow (kJ/h) | 7.477e+009 | 2.822e+009 | 2.609e+006 | -1.788e+007 | 4.348e+004 |

Compositions

Fluid Pkg: All

| Name | Rect Out | Boilup | To Reboiler | To Rect | Propane |
|--------------------------|----------|--------|-------------|---------|---------|
| Comp Mole Frac (Propane) | 0.0002 | 0.9900 | 0.9900 | 0.0002 | 0.9913 |
| Comp Mole Frac (Propene) | 0.9998 | 0.0100 | 0.0100 | 0.9998 | 0.0087 |

| Name | To Condenser | Reflux | Propene | Feed | CGP |
|--------------------------|--------------|--------|---------|--------|--------|
| Comp Mole Frac (Propane) | 0.0000 | 0.0000 | 0.0000 | 0.4000 | 0.0100 |
| Comp Mole Frac (Propene) | 1.0000 | 1.0000 | 1.0000 | 0.6000 | 0.9900 |

Energy Streams

Fluid Pkg: All

| Name | Q-Reboiler | Q-Condenser |
|------------------|------------|-------------|
| Heat Flow (kJ/h) | 4.644e+009 | 4.652e+009 |

Unit Ops

| Operation Name | Operation Type | Feeds | Products | Ignored | Calc. Level |
|----------------|-----------------|--------------|--------------|---------|-------------|
| Reboiler | Reboiler | To Reboiler | Propane | No | 500.0 |
| | | Q-Reboiler | Boilup | | |
| Condenser | Total Condenser | To Condenser | Propene | No | 500.0 |
| | | Q-Condenser | Reflux | | |
| | | Q-Condenser | Q-Condenser | | |
| Stripper | Tray Section | Rect Out | To Reboiler | No | 500.0 |
| | | Boilup | To Rect | | |
| | | Feed | CGP | | |
| Rectifier | Tray Section | Reflux | Rect Out | No | 500.0 |
| | | To Rect | To Condenser | | |



UNIVERSITY OF PETROLEUM
 Calgary, Alberta
 CANADA

Case Name: X:\vamkumar\chandru4.hsc
 Unit Set: SI
 Date/Time: Mon Apr 23 12:18:31 2007

Distillation: T-100 @Main

CONNECTIONS

Inlet Stream

STREAM NAME

Stage

FROM UNIT OPERATION

Q-Reboiler
 Feed

Reboiler
 52 Stripper

Outlet Stream

STREAM NAME

Stage

TO UNIT OPERATION

Propane
 Q-Condenser
 Propene
 CGP

Reboiler
 Condenser
 Condenser
 73 Stripper

MONITOR

Specifications Summary

| | Specified Value | Current Value | Wt. Error | Wt. Tol. | Abs. Tol. | Active | Estimate | Used |
|-------------------|------------------|----------------|-------------|--------------|------------------|--------|----------|------|
| Reflux Ratio | 16.40 * | 1082 | 64.96 | 1.000e-002 * | 1.000e-002 * | Off | On | Off |
| Draw Rate | 351.1 kgmole/h * | 351.3 kgmole/h | 3.273e-004 | 1.000e-002 * | 1.000 kgmole/h * | On | On | On |
| Comp Fraction | 1.000e-002 * | 1.001e-002 | 4.292e-004 | 1.000e-002 * | 1.000e-003 * | On | On | On |
| Comp Fraction - 2 | 0.9900 * | 0.9900 | -9.695e-004 | 1.000e-002 * | 1.000e-003 * | On | On | On |

SPECS

Column Specification Parameters

Reflux Ratio

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

Draw Rate

| | | | | | | | |
|-----------------|---------|----------------------|---------|--------------|-----|--------------|-----|
| Fixed / Ranged: | Fixed | Primary / Alternate: | Primary | Lower Bound: | --- | Upper Bound: | --- |
| Stream: | Propene | Flow Basis: | Molar | | | | |

Comp Fraction

| | | | | | | | |
|-----------------|--------------|----------------------|---------------|--------------|--------|--------------|-----|
| Fixed / Ranged: | Fixed | Primary / Alternate: | Primary | Lower Bound: | --- | Upper Bound: | --- |
| Stage: | 182 Stripper | Flow Basis: | Mole Fraction | Phase: | Liquid | | |
| Components: | Propene | | | | | | |

Comp Fraction - 2

| | | | | | | | |
|-----------------|-------------|----------------------|---------------|--------------|--------|--------------|-----|
| Fixed / Ranged: | Fixed | Primary / Alternate: | Primary | Lower Bound: | --- | Upper Bound: | --- |
| Stage: | 73 Stripper | Flow Basis: | Mole Fraction | Phase: | Liquid | | |
| Components: | Propene | | | | | | |

SUBCOOLING

Condenser

Degrees of Subcooling
 Subcool to

User Variables

PROFILES

General Parameters

Sub-Flow Sheet: T-100 (COL1) Number of Stages: 182 *



UNIVERSITY OF PETROLEUM
Calgary, Alberta
CANADA

Case Name: X:\ramkumarchandru4.hsc

Unit Set: SI

Date/Time: Mon Apr 23 12:18:31 2007

Distillation: T-100 @Main (continued)

Stage Efficiencies

| Stages | Overall Efficiency | Propane | Propene |
|--------------|--------------------|---------|---------|
| 148 Stripper | 1.000 | 1.000 | 1.000 |
| 149 Stripper | 1.000 | 1.000 | 1.000 |
| 150 Stripper | 1.000 | 1.000 | 1.000 |
| 151 Stripper | 1.000 | 1.000 | 1.000 |
| 152 Stripper | 1.000 | 1.000 | 1.000 |
| 153 Stripper | 1.000 | 1.000 | 1.000 |
| 154 Stripper | 1.000 | 1.000 | 1.000 |
| 155 Stripper | 1.000 | 1.000 | 1.000 |
| 156 Stripper | 1.000 | 1.000 | 1.000 |
| 157 Stripper | 1.000 | 1.000 | 1.000 |
| 158 Stripper | 1.000 | 1.000 | 1.000 |
| 159 Stripper | 1.000 | 1.000 | 1.000 |
| 160 Stripper | 1.000 | 1.000 | 1.000 |
| 161 Stripper | 1.000 | 1.000 | 1.000 |
| 162 Stripper | 1.000 | 1.000 | 1.000 |
| 163 Stripper | 1.000 | 1.000 | 1.000 |
| 164 Stripper | 1.000 | 1.000 | 1.000 |
| 165 Stripper | 1.000 | 1.000 | 1.000 |
| 166 Stripper | 1.000 | 1.000 | 1.000 |
| 167 Stripper | 1.000 | 1.000 | 1.000 |
| 168 Stripper | 1.000 | 1.000 | 1.000 |
| 169 Stripper | 1.000 | 1.000 | 1.000 |
| 170 Stripper | 1.000 | 1.000 | 1.000 |
| 171 Stripper | 1.000 | 1.000 | 1.000 |
| 172 Stripper | 1.000 | 1.000 | 1.000 |
| 173 Stripper | 1.000 | 1.000 | 1.000 |
| 174 Stripper | 1.000 | 1.000 | 1.000 |
| 175 Stripper | 1.000 | 1.000 | 1.000 |
| 176 Stripper | 1.000 | 1.000 | 1.000 |
| 177 Stripper | 1.000 | 1.000 | 1.000 |
| 178 Stripper | 1.000 | 1.000 | 1.000 |
| 179 Stripper | 1.000 | 1.000 | 1.000 |
| 180 Stripper | 1.000 | 1.000 | 1.000 |
| 181 Stripper | 1.000 | 1.000 | 1.000 |
| 182 Stripper | 1.000 | 1.000 | 1.000 |
| Reboiler | 1.000 | 1.000 | 1.000 |

SOLVER

Column Solving Algorithm: HYSIM Inside-Out

Solving Options

1000 *

Accelerate K Value & H Model Parameters:

Off

Maximum Iterations: 1.000e-05

Equilibrium Error Tolerance: 5.000e-004

Heat/Spec Error Tolerance: On

Save Solutions as Initial Estimate: Simple K

Super Critical Handling Model: Low

Trace Level: Off

Damping Parameters

Init from Ideal K's:

Azeotrope Check:

Off

Initial Estimate Generator Parameters

Off

Fixed Damping Factor:

1

Iterative IEG (Good for Chemicals):

SIDE STRIPPERS



UNIVERSITY OF PETROLEUM
Calgary, Alberta
CANADA

Case Name: X:vamkumarchandru4.hsc

Unit Set: SI

Date/Time: Mon Apr 23 12:18:31 2007

Distillation: T-100 @Main (continued)

SIDE STRIPPERS

SIDE RECTIFIERS

PUMP AROUNDS

VAP BYPASSES

RATING

Tray Sections

| Tray Section | Stripper | Rectifier |
|--------------------------------|------------|------------|
| Tray Diameter (m) | 2.600 | 1.500 |
| Weir Height (m) | 5.000e-002 | 5.000e-002 |
| Weir Length (m) | 2.080 | 1.200 |
| Tray Space (m) | 0.5000 | 0.5000 |
| Tray Volume (m3) | 2.655 | 0.8836 |
| Disable Heat Loss Calculations | No | No |
| Heat Model | None | None |
| Rating Calculations | No | No |
| Tray Hold Up (m3) | 8.836e-002 | 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) |
|---------------|----------------|---------------------|
| | 1931 kPa | 0.0000 kPa |
| Condenser | 1931 kPa | 0.7835 kPa |
| 1_ Rectifier | 1931 kPa | 0.7835 kPa |
| 2_ Rectifier | 1932 kPa | 0.7835 kPa |
| 3_ Rectifier | 1933 kPa | 0.7835 kPa |
| 4_ Rectifier | 1934 kPa | 0.7835 kPa |
| 5_ Rectifier | 1934 kPa | 0.7835 kPa |
| 6_ Rectifier | 1935 kPa | 0.7835 kPa |
| 7_ Rectifier | 1936 kPa | 0.7835 kPa |
| 8_ Rectifier | 1937 kPa | 0.7835 kPa |
| 9_ Rectifier | 1938 kPa | 0.7835 kPa |
| 10_ Rectifier | 1938 kPa | 0.7835 kPa |
| 11_ Rectifier | 1939 kPa | 0.7835 kPa |
| 12_ Rectifier | 1940 kPa | 0.7835 kPa |
| 13_ Rectifier | 1941 kPa | 0.7835 kPa |
| 14_ Rectifier | 1942 kPa | 0.7835 kPa |
| 15 Rectifier | | |



UNIVERSITY OF PETROLEUM
Calgary, Alberta
CANADA

Case Name: X:\ramkumar\chandru4.hsc

Unit Set: SI

Date/Time: Mon Apr 23 12:18:31 2007

Distillation: T-100 @Main (continued)

PROPERTIES

| Name | Feed @Main | Propane @Main | PGP @Main | CGP @Main |
|--|------------|---------------|-----------|-----------|
| Cv (Semi-Ideal) (kJ/kgmole-C) | 89.94 * | 157.6 * | 80.17 * | 136.6 * |
| Mass Cv (Semi-Ideal) (kJ/kg-C) | 2.097 * | 3.575 * | 1.905 * | 3.245 * |
| Cv (kJ/kgmole-C) | 66.48 * | 113.9 * | 60.70 * | 97.17 * |
| Mass Cv (kJ/kg-C) | 1.550 * | 2.583 * | 1.442 * | 2.308 * |
| Cv (Ent. Method) (kJ/kgmole-C) | — | — | 60.69 * | 132.9 * |
| Mass Cv (Ent. Method) (kJ/kg-C) | — | — | 1.442 * | 3.156 * |
| Cp/Cv (Ent. Method) | — | — | 1.458 * | 1.091 * |
| Reid VP at 37.8 C (kPa) | 1494 * | — | — | — |
| True VP at 37.8 C (kPa) | 1500 * | 1321 * | 1583 * | 1581 * |
| Liq. Vol. Flow - Sum(Std. Cond) (m3/h) | 49.79 * | 21.01 * | 28.25 * | 0.5384 * |

SUMMARY

Flow Basis: Molar The recovery option is selected

Feed Composition

| Feed | | | |
|----------------------|----------|--|--|
| Flow Rate (kgmole/h) | 600.0000 | | |
| Propane | 0.4000 | | |
| Propene | 0.6000 | | |

Feed Flows

| Feed | | | |
|----------------------|----------|--|--|
| Flow Rate (kgmole/h) | 600.0000 | | |
| Propane (kgmole/h) | 240.0000 | | |
| Propene (kgmole/h) | 360.0000 | | |

Products

Flow Basis: Molar The recovery option is selected

Product Compositions

| Propene | CGP | Propane | |
|----------------------|----------|---------|----------|
| Flow Rate (kgmole/h) | 351.2625 | 6.6897 | 242.0478 |
| Propane | 0.0000 | 0.0100 | 0.9913 |
| Propene | 1.0000 | 0.9900 | 0.0087 |

Product Flows

| Propene | CGP | Propane | |
|----------------------|------------|----------|------------|
| Flow Rate (kgmole/h) | 351.2625 * | 6.6897 * | 242.0478 * |
| Propane (kgmole/h) | 0.0001 * | 0.0669 * | 239.9330 * |
| Propene (kgmole/h) | 351.2625 * | 6.6228 * | 2.1147 * |

Product Recoveries

| Propene | CGP | Propane | |
|----------------------|----------|---------|----------|
| Flow Rate (kgmole/h) | 351.2625 | 6.6897 | 242.0478 |
| Propane (%) | 0.0000 | 0.0279 | 99.9721 |
| Propene (%) | 97.5729 | 1.8397 | 0.5874 |

COLUMN PROFILES

Reflux Ratio: 1082 Reboil Ratio: 1659 The Flows Option is Selected Flow Basis: Molar

* Specified by user.

Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK

Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK

Rating

Vessel Sizing

| Vessel | Reboiler | Condenser |
|---------------------------|--------------------------|--------------------------|
| Diameter [m] | 1.193 | 1.193 |
| Length [m] | 1.735 | 1.789 |
| Volume [m ³] | 2.000 | 2.000 |
| Orientation | Horizontal | Horizontal |
| Vessel has a Boot | <input type="checkbox"/> | <input type="checkbox"/> |
| Boot Diameter [m] | <empty> | <empty> |
| Boot Length [m] | <empty> | <empty> |
| Hold Up [m ³] | 1.000 | 1.000 |

Design Parameters Side Ops **Rating** Worksheet Performance Flowsheet Reactors Dynamics

Delete Column Environment... Run Reset Converged Update Outlets Ignored

Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK

Rating

Tray/Packed Section Sizing

| Tray/Packed Section | Stripper | Rectifier |
|--------------------------------------|-------------------------------------|-------------------------------------|
| Uniform Section | <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> |
| Internal Type | Sieve | Sieve |
| Diameter [m] | 2.600 | 1.500 |
| Tray/Packed Space [m] | 0.5000 | 0.5000 |
| Tray/Packed Volume [m ³] | 2.655 | 0.8836 |
| Disable Heat Loss Calcs | <input type="checkbox"/> | <input type="checkbox"/> |
| Heat Model | None | None |
| Rating Calculators | <input type="checkbox"/> | <input type="checkbox"/> |
| Hold Up [m ³] | 8.836e-002 | 8.836e-002 |
| Weeping Factor | 1.000 | 1.000 |

For more detailed and tray by tray information see the individual tray/packed section in the Column Environment

Design Parameters Side Ops **Rating** Worksheet Performance Flowsheet Reactors Dynamics

Delete Column Environment... Run Reset Converged Update Outlets Ignored

Sensitivity analysis:

- Recovery
- Pressure VS Tray position from top
- Temperature VS tray position from top
- Column properties VS tray position
- Flow VS tray position from top
- K-Value VS tray position from top
- Composition VS tray position from top

Column: T-100 / COL1 Fluid Pkg: Basis-1 / SRK

Column T-100 / COL1 Fluid Pkg: Basis-1 / SRK

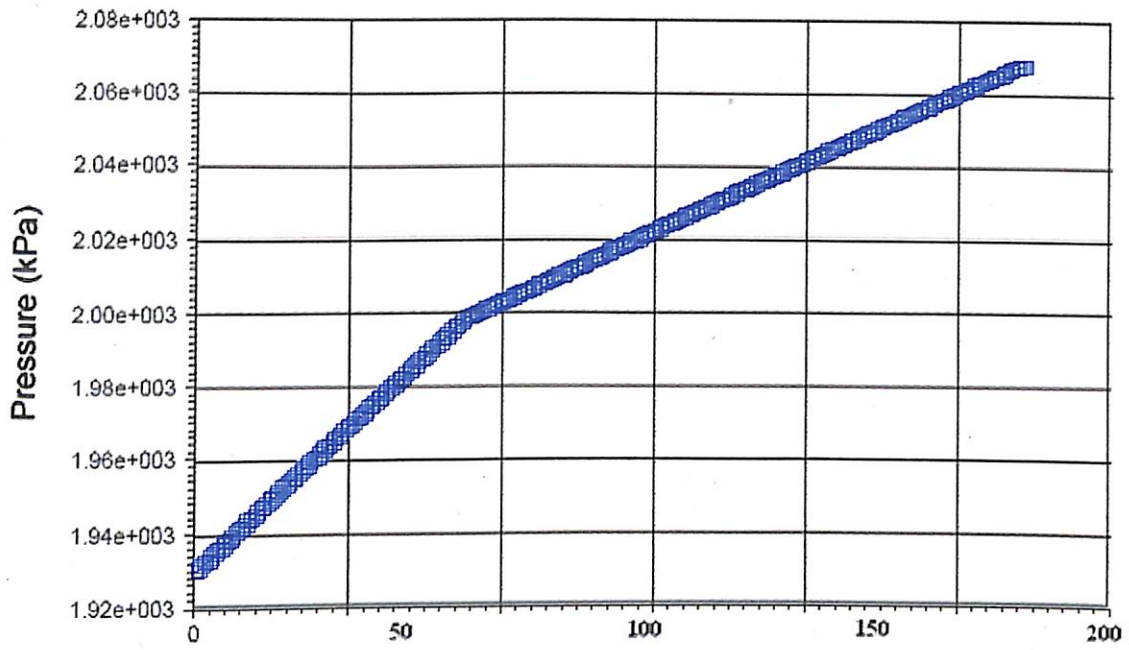
| Feeds | | Feed | | | |
|----------------------|--|-------|--|--|--|
| Flow Rate (kgmole/h) | | 600.0 | | | |
| Propane (kgmole/h) | | 240.0 | | | |
| Propene (kgmole/h) | | 360.0 | | | |

| Product | | Propane | CGP | Propene |
|----------------------|--|----------|---------|----------|
| Flow Rate (kgmole/h) | | 351.1689 | 15.6651 | 233.3650 |
| Propane (%) | | 1.1167 | 2.6005 | 96.3929 |
| Propene (%) | | 96.0025 | 2.6293 | 1.5636 |

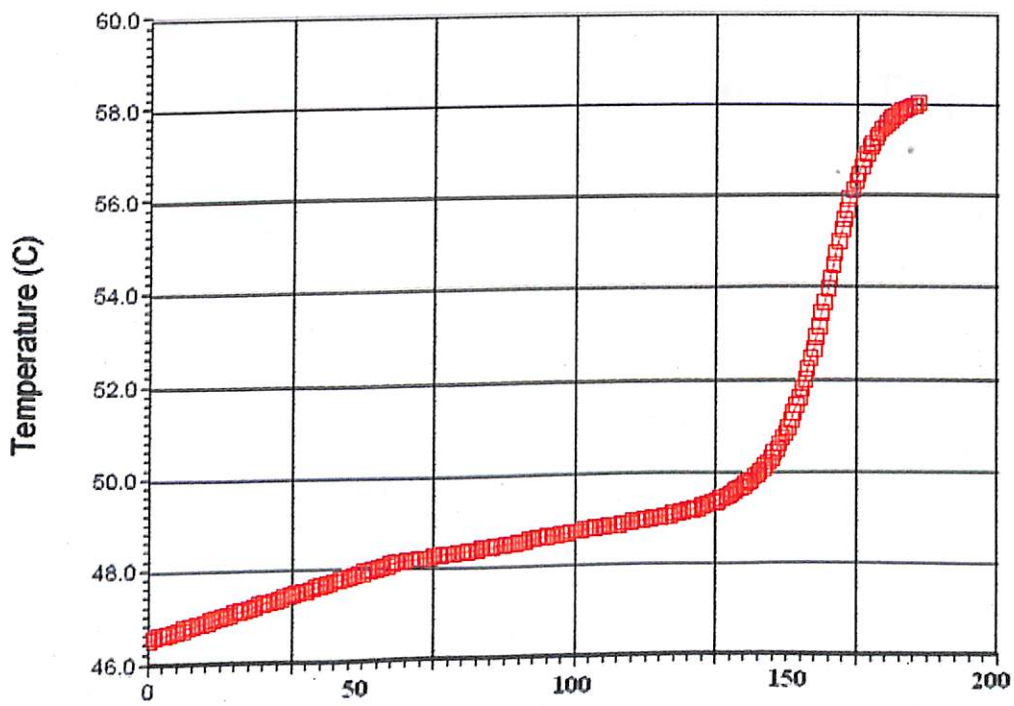
Composition
 Flow
 Recovery
 Molar
 Mass
 Liquid

Design Parameters Side Ops Rating Worksheet **Performance** Flowsheet Reactions Dynamics
 Delete Column Environment... Run Escort Converged Update Outlet: Ignored

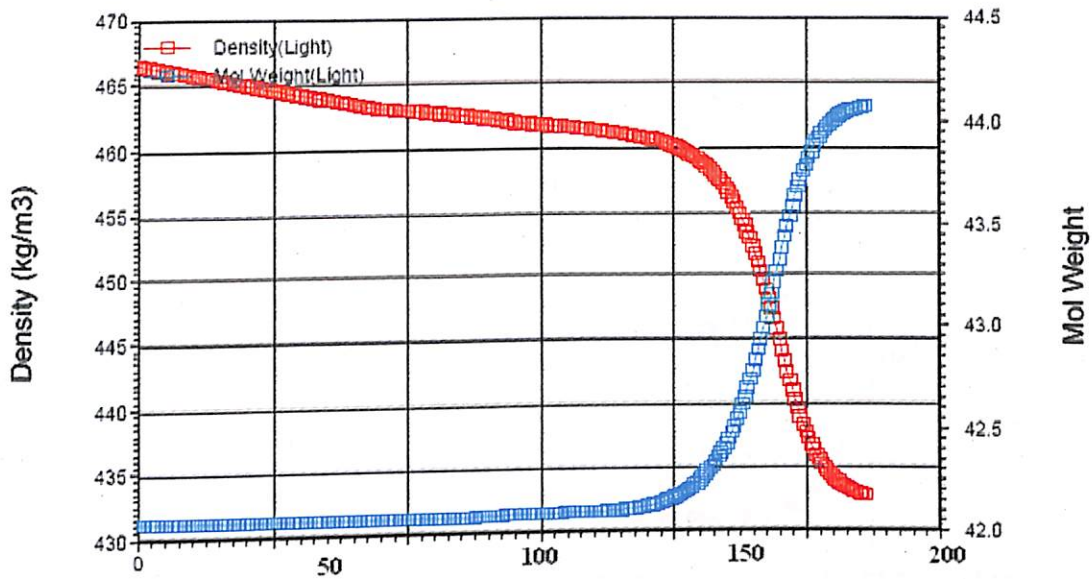
Pressure VS Tray Position from Top



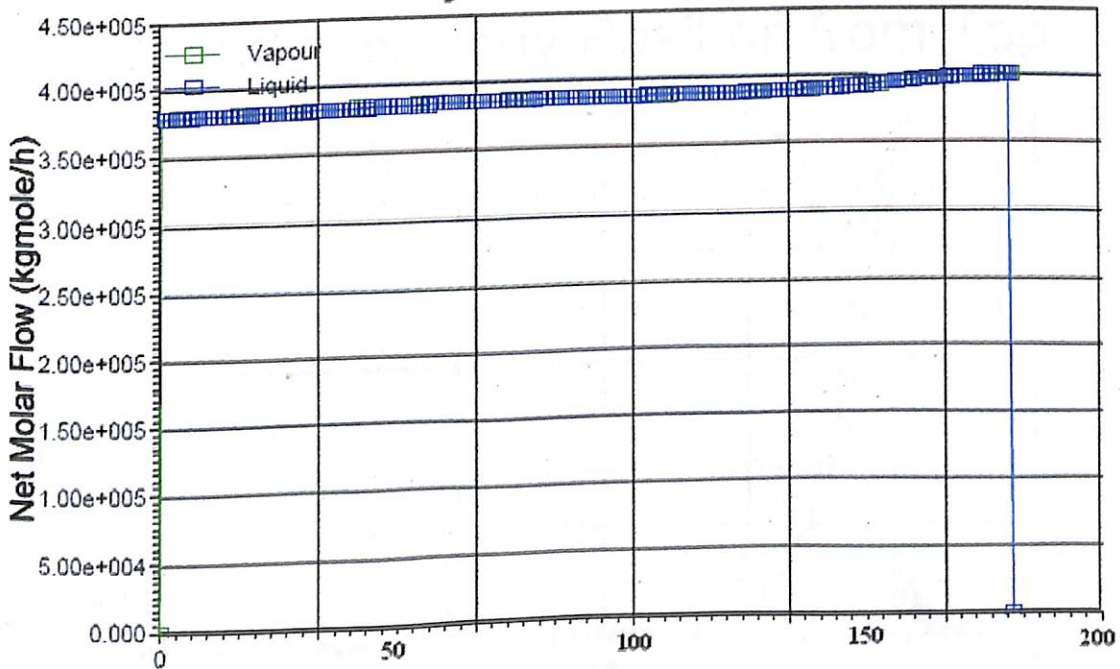
Temperature VS Tray position from the Top



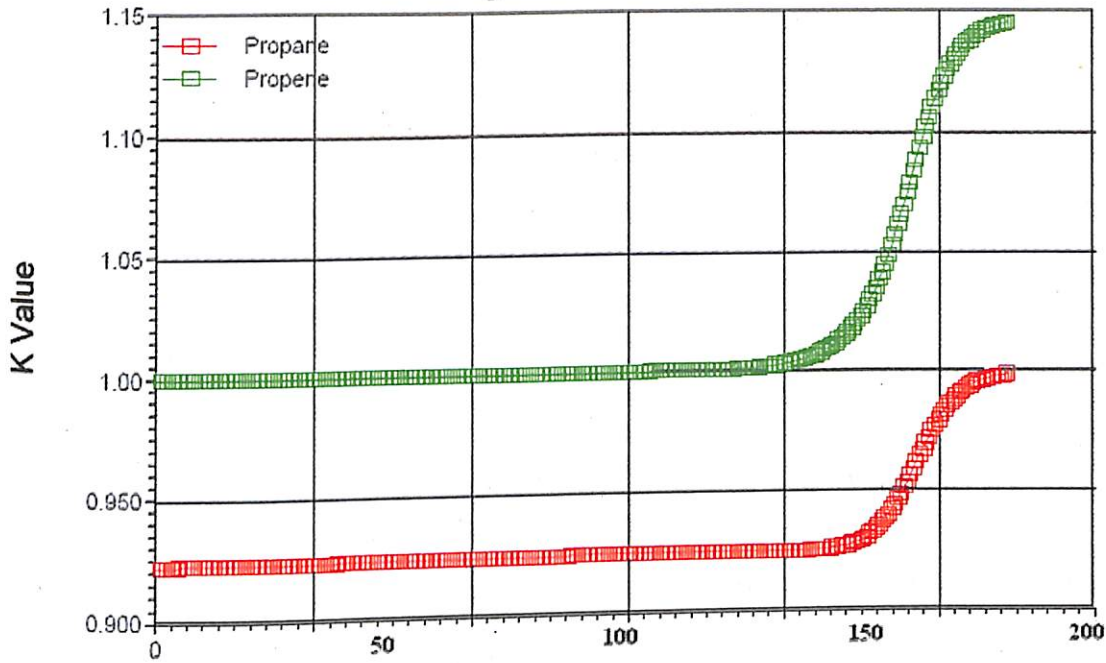
Column Properties VS Tray Position



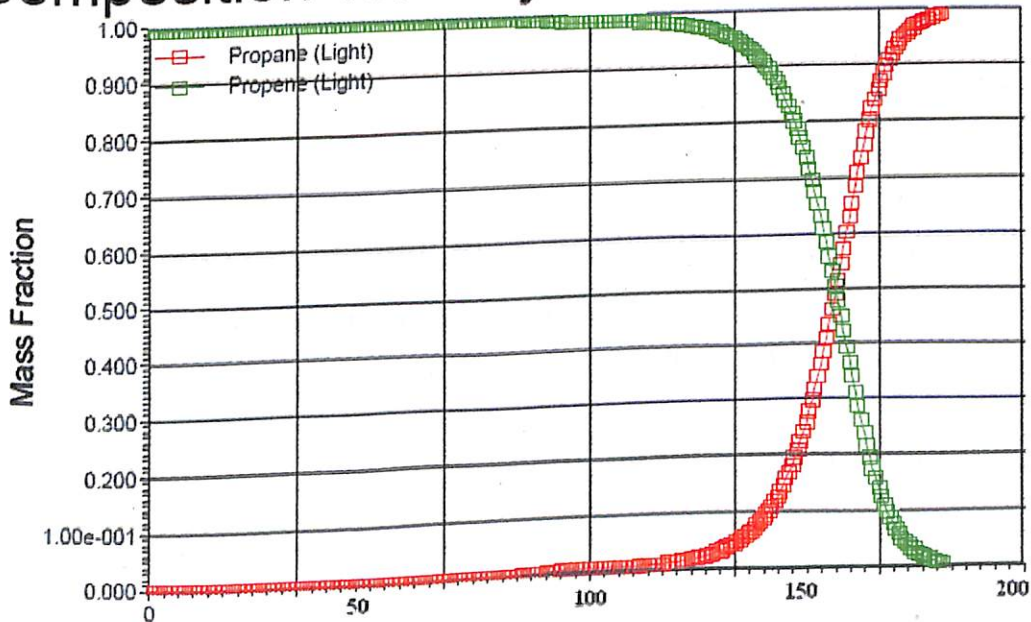
Flow vs. Tray Position from Top



K-Value vs. Tray Position from Top



Composition vs. Tray Position from Top



6.1 Results and Discussion:

The simulation result obtained from ASPEN HYSYS 2004 Version and the resulting analysis has been studied under different conditions.

- ✓ Steady state simulation of column is done using HYSYS, for predicting the mixture properties; an appropriate thermodynamic model (fluid package) is selected based on the decision chart and recommendations given in the HYSYS documentation.
- ✓ One feed stream taken with only two components (propane & propylene) are taken and remaining traces are neglected.
- ✓ Total condenser is chosen because the feed contains non-condensable components.
- ✓ While simulating, we consider manipulated variables as reflux ratio, No. of stages, pressure and controlled variables as top and bottom product composition.
- ✓ The specification under which the splitter was converged is reflux ratio, draw rate (D), Composition fraction. The specifications should be selected such that the degree of freedom should be zero, which is a basic condition for simulation process.
- ✓ Instead of shortcut method, we have chosen rigorous method. Inside- out method is chosen for mathematical solution.
- ✓ In this case study, propylene product purity of 98.5% was obtained with a recovery of 96%.
- ✓ Finally, in this analysis, we didn't consider any economics; instead we focused mainly on recovery and product purity.

6.2 LATEST DEVELOPMENTS IN PROPYLENE RECOVERY UNIT:

Propylene is one of basic feed stocks and is used in huge quantities in petrochemical industry. The separation of propylene-propane mixtures have been performed by highly energy intensive distillation process at 40⁰ C and 240 psig (16 kg/cm²) in a column of 220 trays because of the close relative volatility of the components. A number of alternative methods have been investigated for olefin/paraffin separation.[4]

1. Possible operating schemes for Propylene/Propane Fractionator:(Ref Fig :)

- Scheme A: The column is operated at a pressure high enough for the overhead to be condensed by cooling water.
- Scheme B: The process is operated with refrigeration, at a level such that the heating medium is cooling water at 30⁰C.
- Scheme C: The process utilizes vapor recompression distillation, with only mechanical work being added to the system.
- Scheme D: This is alternative form of vapor-recompression distillation, in which the bottom liquid is expanded for refrigerant value, to condense the over head stream, and is then recompresses as reboiler vapor.

Reference:

- Recent developments in chemical process and plant design by Y.A.LIU & HENRY A. MCGEE, JR (chapter-3, Title: Energy efficient separation process design, page no: 71 – 97).

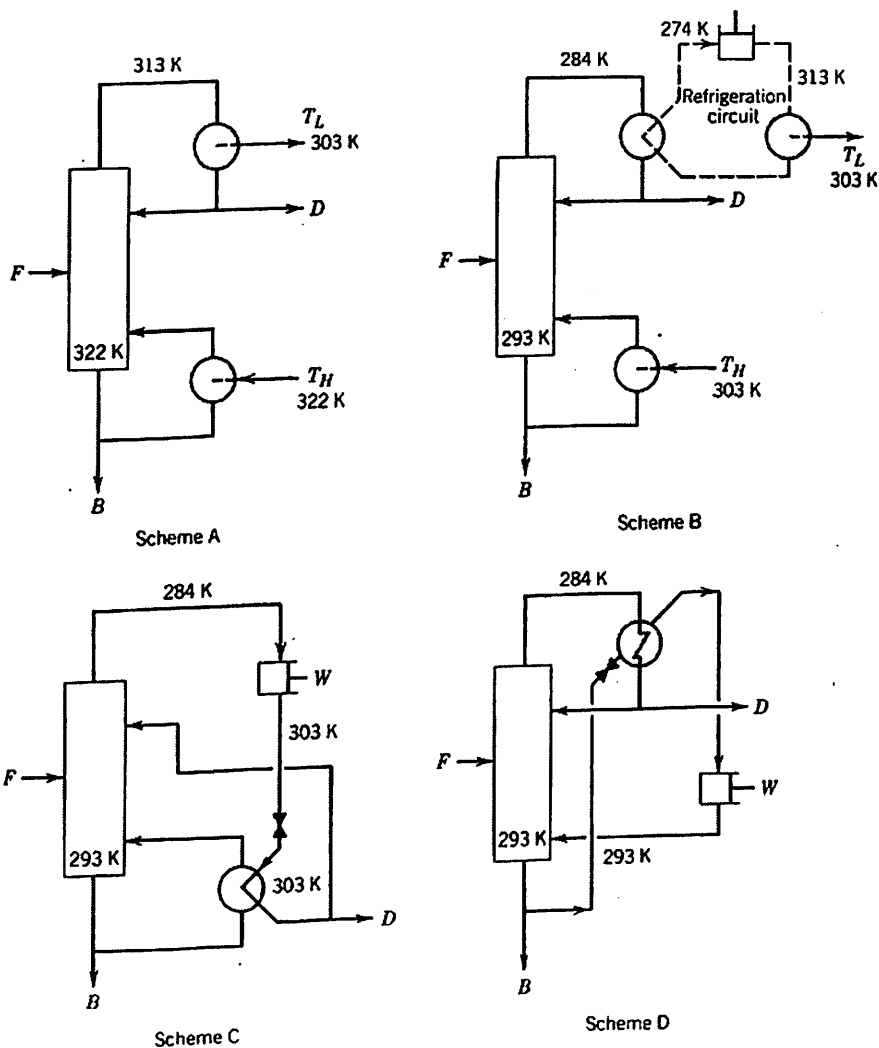


FIGURE 3.4 Possible operating schemes for propylene/propane fractionation.

2. Propylene separation from C₃ fractionator feed gas by pressure swing adsorption:

In this work, the separation of propylene-propane mixtures was performed by pressure swing adsorption using a g-complexation sorbent (AgNO₃/aluminasilica). A three bed and a six step PSA cycle was used for propylene separation from C₃ fractionator feed gas in naphtha cracker center. The PSA unit was operated in the pressure range of 35mmHg to 980 mmHg (0.048 – 1.35 kg/cm²) and the performance was examined with the adsorber temperature range of 25 to 80^o C. the best PSA performance was shown at the adsorber temperature of 70^o C. In this case, propylene product purity of 99.5 % was obtained with the recovery of 96 % and the productivity of 3.56 gmol/(kg.h).

Reference:

- separation process research center, Korea institute of energy research, south Korea
- Chemical process technology team, SK Corporation, South Korea.

3. Vacuum swing adsorption process for separating propylene and propane:

A vacuum swing adsorption process is provided for the separation of propylene from feed stream comprising propylene and propane using an adsorbent comprising AIPO-14. To produce a high purity propylene product stream at high recovery. The vacuum swing adsorption process of the present invention can be employed in a variety of petroleum refining and petrochemical processes to purify and separate propylene from the mixtures of propylene and propane alone or in combination with fractionation.

Reference:

- United States patent 6296688

4. Utilization of Hybrid membrane in propylene separation :

Membrane separations, which are generally less energy intensive than conventional separations, have been considered promising alternatives for some industrial applications. One of the examples considered is ethylene production in which more than 70% of the energy required is consumed in the purification sections.

A very critical process located in the separation sections of the ethylene plant is the propane/propylene fractionation. This process is currently based on distillation technology that is both expensive and energy intensive. In general, the separation of a low relativity mixture, such as propane/propylene, by using distillation alone is a critical task. It requires large number of equilibrium trays and high reflux ration. A reflux ratio of 20 and up to 200 trays is required for such a separation. However, the application of new technologies, such as selective membrane, may enhance this process.

To produce polymer grade propylene, the membrane alone cannot perform the separation and a hybrid distillation/membrane system is required. Furthermore, the use of simple diffusion membranes for such a process is uneconomical because of the slow transfer rates and selectivity in separation. However, using the facilitated transport (FT) scheme, membranes can make this process feasible. In the FT scheme, the simple diffusion processes coupled with a chemical reactant that reversibly binds with one of the species to be separated which increases the net transport rate.

Hybrid distillation with FT membranes has been evaluated recently for the propane/propylene separation. In the study, the conventional distillation column for propane/propylene is coupled in different configurations with a facilitated transport membrane to form a hybrid system. Simulation and optimization processes are performed for each hybrid configuration. In the process of the simulations, the design parameters, such as membrane pressure ratio, carrier concentration, and reflux ratio are considered. The economic effect of the main design variables on the hybrid system is examined through

parametric studies. For each case of parametric study, design and cost of all equipment associated with each hybrid system are evaluated. The ultimate design is based on economic comparisons. Economic criteria such as processing costs and NPV (net Present value) are used to evaluate the profitability. The hybrid separation system provides considerable reduction in both capital and operating costs.

Reference:

“Membrane /distillation hybrid design for propane/propylene separation” presented at the AIChE spring national meeting new Orleans.

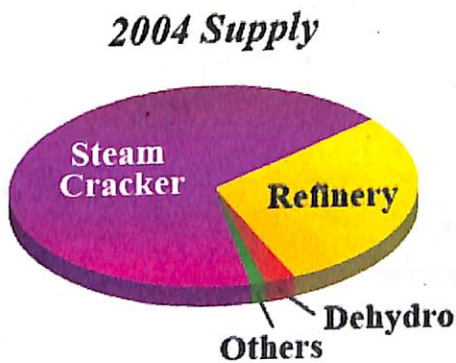
5. Extractive Distillation with a polar solvent such as furfural or an aliphatic nitrile that will reduce the volatility of propylene.(Ref: U.S. patent 2,588,056)[7]
6. Adsorption with silica gel or a zeolite that will selectively adsorb propylene(Ref: J.Am.chem.soc, 72, 1153-1157(1950))
7. Facilitated transport membranes using impregnated silver nitrite to carry propylene selectively through the membrane.(Ref: recent developments in separation science)

6.3 Demand / Supply of propylene:

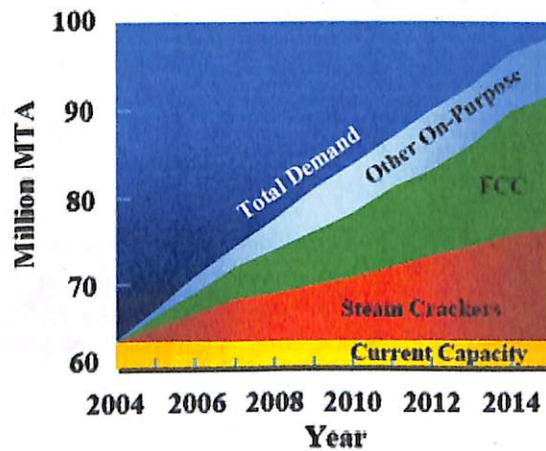
Propylene production is projected to come from a number of sources, both refinery and petrochemical-complex based. On the refining side, increased propylene production from FCC units is expected to be a major contributor to the on-purpose requirement. It is expected that this FCC production will come from revamps of existing FCC units as well as an increasing petrochemical focus in new FCC units installed to meet transportation fuel market demands.[16]

On the petrochemical side, there are more alternative routes to propylene available than ever before. These alternatives include propane dehydrogenation, methanol-to-olefins, and olefin conversion including metathesis and olefin cracking processes. Each of these alternatives can offer competitive economics in certain situations.

*Propylene Supply and Demand
Polymer Grade & Chemical Grade*



Source: CMAI



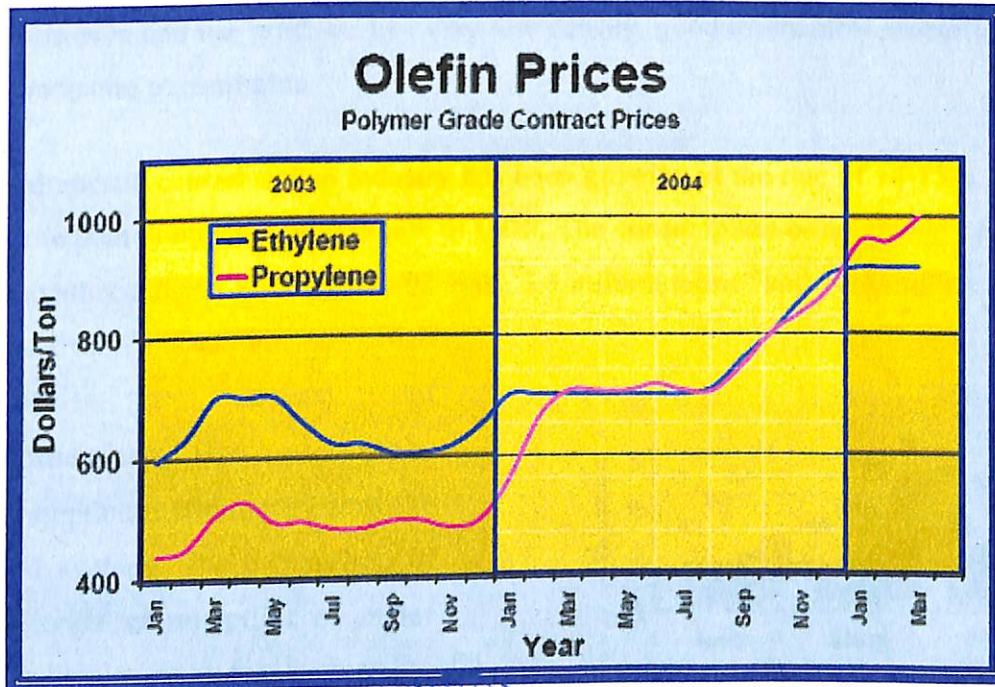
Demand growth expected will exceed 4.5% - 5.0% per year in the next few years.

Demand in Asia will be stronger, growing at nearly 6% per year.

Present price of the propylene grade was as follows:[17]

| Grade of Propylene | Dollars(\$) per Pound |
|-------------------------------|-----------------------|
| Polymer grade propylene(PGP) | 0.225 |
| Chemical grade propylene(CGP) | 0.210 |

Ethylene/Propylene Price relationships:



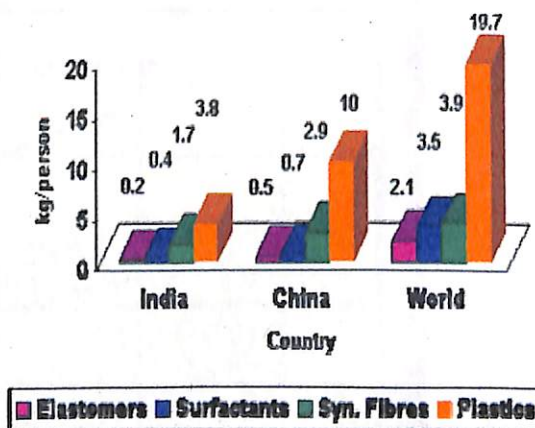
Strong demand for propylene derivatives is one of the keys:

- Polypropylene
- Acrylonitrile
- Oxo chemicals
- Propylene oxide
- Cumene
- Isopropyl alcohol
- Polygas chemicals

Polypropylene accounts for more than 60% of propylene demand due to its favorable properties in end use products like very low density, good mechanical properties, and low moisture transmission.

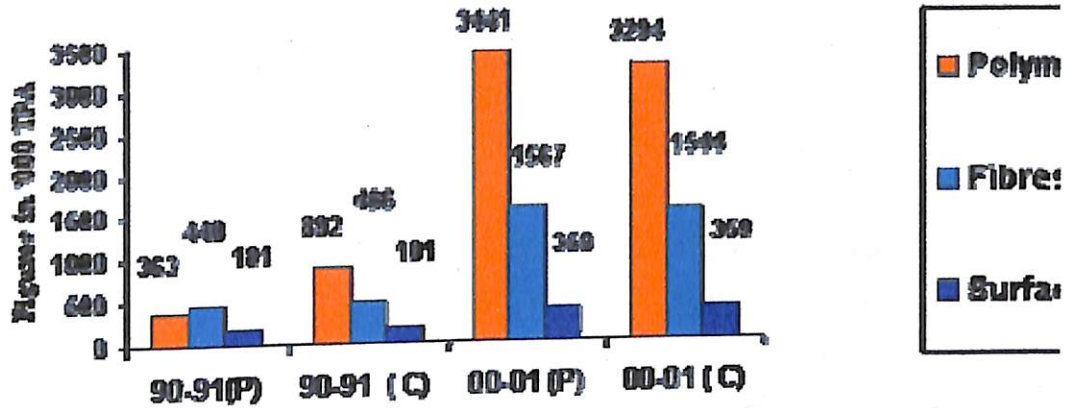
The domestic petrochemical industry has been growing at the rate of 14-15%, which is more than double the growth rate of GDP. The consumption of commodity plastics and synthetic fibres during 2001-02 was 3.8 million tonnes and 1.65 million tonnes respectively. Despite very high

growth in demand of petrochemicals, the per capita consumption is still much below the world average. The comparison of per capita consumption of major petrochemical segments is given in Figure 1 : Per Capita Consumption of Petrochemicals

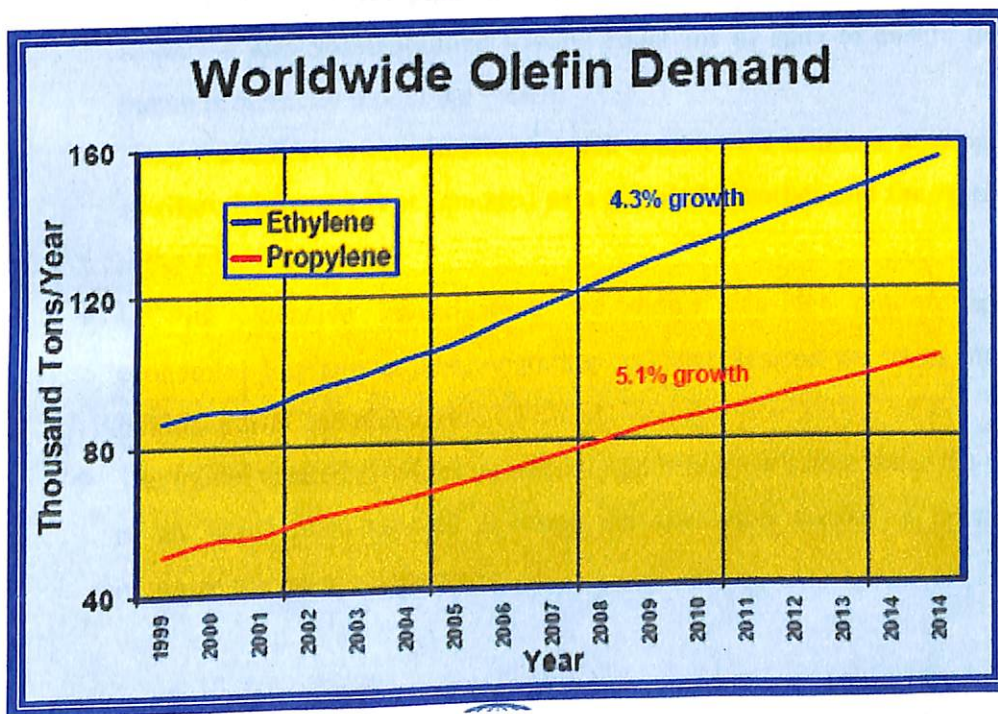


The production and consumption of major petrochemicals namely polymers, synthetic fibre and surfactants are in Figure 3

Figure 3 Trends in Production and Consumption of Petrochemicals.



Driven by high polypropylene and other propylene derivative demand, propylene growth rate will exceed ethylene growth rate.



6.4 Conclusion & Recommendation:

- ❖ The C₃ splitter of a commercial Petrochemical complex was modeled and simulated from plant tests using HYSYS and has been presented. The various important parameters of the column from the results of simulation were studied and compared at the following conclusion.
- ❖ The project was illustrated on the challenging problems posed by the C₃ splitter for which it was found that a classical plant test was not feasible.
- ❖ The procedure is based on the premise that a reliable steady state simulation of the process and every variable that participates in the scheme is developed.
- ❖ A propylene-propane splitter is generally an easy column to converge. However, the critical factor in producing good results is not the ease of solution, but rather the accurate prediction of the relative volatility of the two key components. Special consideration was given to these components, along with others, in developing the binary interaction coefficients for the Peng Robinson and Soave Redlich Kwong equations of state to ensure that these methods correctly model the system.
- ❖ Here, the splitter is simulated which will contain two columns, a stripper and a rectifier. The stripper is operated as a reboiled absorber and the rectifier is a refluxed absorber.
- ❖ In this extensive investigation, we didn't consider optimization (i.e., economics like annual cost, operating cost etc). Instead we focus mainly on product purity and recovery.
- ❖ The model created provides us with an opportunity to know about the working of an actual plant as well as study the alternative modes of operation or optimize the existing operation.

NOMENCLATURE

- A= general stream designation; moles, weight, or volume per unit time.
B= bottom product rate; moles, weight, or volume per unit time.
C= number of components; moles, weight, or volume per unit time.
D=overhead product; moles, weight, or volume per unit time.
F= upper feed rate; moles, weight, or volume per unit time.
 $K_i = y_i / x_i$ = equilibrium distribution coefficient for component i
 $L_{N+1} = RD$ = liquid phase entering stage N;
M= number of theoretical plates below the feed stage
M+1 = Feed stage
n = subscript referring to any stage
N = total number of theoretical stages including reboiler (if it is a theoretical stage) and the feed stage but excluding the condenser.
 N_c = independent restricting variables
 N_v = total number of variables which the designer must consider.
 N_i = degrees of freedom; variance; number of design variables which the designer must arbitrarily specify.
q = general designation for a heat system.
 Q_c = heat removed in the condenser
 Q_r = heat input to reboiler
R = external reflux ratio
S = side stream rate; moles, weight, or volume per unit time.
V = light phase rate; moles, weight, or volume per unit time.
-
-

References

1. Lek C.M., Rangaiah G.P and Hidajat.K., Distillation: Revisiting Some Rules of Thumb, *chemical engineering*, pp. 50-55, September, 2004.
2. G.P Rangaiah, Yue C.T, K. Hidajat., Optimization of Complex Distillation Cloumns, *chemical engineering journal*, pp. 60-64, September, 2006.
3. D.N. Saraf, Vineet Kumar, Anuj Sharma, S.Ganguly, Dept. of Chem.Engg, IIT, Kanpur., A Crude distillation unit model suitable for online applications, *fuel processing technology*73(2001) 1-21., ELSEVIER
4. Fair,J.R.,”Energy efficient separation process design”, *Recent developments in chemical process and design*, Y.A.Liu, John Wiley& sons(1987).
5. Henry Z. Kister, *Distillation Operation*, chp-4 *Rigorous distillation calculations.*, McGraw-Hill(1990).
6. Buford D. Smith, *Design of Equilibrium stage processes*, chapter-3 Design variables., McGraw Hill.
7. J.D Seader & Ernest.J.Henley, *Seperation process Principles*, chapter -1,2,9 & 10, John Wiley & Sons.
8. Apllied case study to a propylene/propane splitter, Scanraff Refinery in Lysekil, Sweden., Authors: Nicholas Alsop & Jose Maria Ferrer
9. HYSYS Tutorials on Propylene/Propane Splitter collected from ASPEN TECH(www.aspentech.com) and Chemical Engineers Resource Page, Forum,(www.cheresources.com).
10. S K Masud Hossain & M kanga Sabapathy., Modeling & Simulation of binary distillation column., *Chemical Engineering World journal.*,pp. 57-59, September 2006.
11. Robert H. Perry, *Perry's chemical Engineer's Handbook.*, Distillation , chp 13 (13-49); 7th Edition Mc-Graw Hill.
12. R.K Sinnott, *Chemical Engineering Design*, COULSON & RICHARDSON'S CHEMICAL ENGINEERING SERIES,P.P 350-352, Volume- 6, fourth Edition.

13. Powerful process simulation technology, PROMAX, Property packages
14. "A comparison of the Peng Robinson and Soave Redlich kwong equation of state using a non zero pressure based mixing rule for the prediction of high pressure and high temperature phase equilibria". Authors: Chorng H. Twu*, John E. Coon, and David Bluck, *Simulation Sciences Inc., 601 Valencia Avenue, Brea, CA 92823 (USA)*, Source: Internet
15. J. Mark Houdek & James Andersen "ON-PURPOSE" PROPYLENE – TECHNOLOGY DEVELOPMENTS, UOP. Presented at the ARTC 8th Annual Meeting, 29-April-2005, Kuala Lumpur.
16. George M. Intille, V.P, SRI consulting, "Propylene in asia growing demand and issues in supply", Asia Petrochemical Industry Conference (APIC), Yokohama, Japan, May 19, 2005.
17. R.W Gaikwad & A.K Chauhan, "*Computer aided design & dynamic simulation of distillation column*", pp. 74-86, *Chemical engineering world*, December 2006.