Simulation Studies of Divided Wall Distillation Column

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DECLARATION

I hereby declare that thesis entitled **"Simulation studies of Divided Wall Distillation Column"**, is an authentic record of my own work carried out as per the requirements for the award of the degree of M.Tech. (Chemical Engineering) at Thapar University, Patiala, under the guidance of Mr. V. K. Sangal (Assistant Professor, CHED) during July 2011 to July 2012.

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ABSTRACT

The divided wall column (DWC) system is a promising energy-saving alternative for separating multi-component mixtures. The innovation is in the structure of this equipment, namely there is a wall in it which divides the space in the tower so the feed and the side stream-product zones are separated. Divided wall column can effectively reduce energy requirement by up to 30% and also lowers engineering and hardware costs compared with conventional direct and indirect distillation sequences. Conventional ternary separations progressed from the (in-) direct sequences to thermally coupled columns such as Petlyuk configuration, and later to the DWC compact design that integrates the two distillation columns into one shell. However at the same time this integration also leads to changes in the control and operating mode. Despite its potential to make major savings in energy and capital costs in distillation, it has not been widely used in practice. One of the major fears in applying the technology is uncertainty regarding the control and operation of the arrangement. A variety of controllers are used for binary distillation columns, only a few control structures were studied for DWC. In most of the cases multi-loop PID controllers were used to steer the system to the desired steady state.

Simulation of a DWC is a difficult task, as it involves a number of variables and a highly nonlinear problem. The steady state and dynamic simulation of DWC were done in ASPEN PLUS and ASPEN dynamics respectively.

The system under study was ternary separation of the mixture benzene-toluene-xylene (BTX) in DWC. The simulations were carried out by varying the operational parameters assuming the structural variables as constant and the optimum values of vapor split and liquid split were obtained for the minimizing the reboiler duty. At steady state, the optimum liquid split and vapor split were found to be 0.603 and 0.45 respectively, for the separation of BTX ternary mixture. At optimum conditions the minimum reboiler duty was found to be 15770 kW.

A conventional control structure based on PID control loops was used as a control basis. From the study of the control and dynamics of a DWC, it was found that the control structure enhanced by adding an extra loop controlling the heavy component composition in the top of the pre-fractionator, by using the liquid split as an additional manipulated variable, thus implicitly achieving minimization of energy requirements. The results of the dynamic simulations show that the concentration of the components in the product streams returned to the set point soon after the disturbance in form of change in feed flow rate or the feed composition was introduced.

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NOMENCLATURE AND ABBREVIATIONS

x_D: Distillate Purity
x_B: The Bottom Purity
x_S: Side Stream Purity
z: feed composition
F: Feed flow rate
S: Side Stream Flow Rate
V: Vapor Boil Up
L: Reflux Rate
D: Distillate Flow Rate
B: Bottom Product Rate
d: diameter of a block
l: length of a block
N_T: number of stages
α_{ij}: relative volatility
y_i: mole fraction of light in the vapor phase
y_j: mole fraction of heavy in the vapor phase
x_i: mole fraction of light in the liquid phase
x_j: mole fraction of heavy in the liquid phase
ΔL_F: change in liquid flow rate at the feed stage
ΔV_F: change in vapour flow rate at the feed stage
ΔH^{vap}: latent heat of vaporization
$h_{v,sat}$: enthalpy of saturation
h_f: enthalpy of feed
q: feed liquid fraction
N_{min}: minimum number of stages
x_{i1}: mole fraction of light at the top stage
x_{j1}: mole fraction of heavy component at top stage
$x_{j\,N+1}$: mole fraction of light at the bottom stage
$x_{j\,N+1}$: mole fraction of heavy component at bottom stage
α_m: mean relative volatility
$(\alpha_{ij})_N$: relative volatility of light and heavy key at bottom stage
$(\alpha_{ij})_1$: relative volatility of light and heavy key at top stage
P_j^S: vapor pressure of a component
B_j: Antoine constant to calculate the vapor pressure
C_j: Antoine constant to calculate the vapor pressure
T: Temperature
d_i : light component distillate flow
d_j : heavy component distillate flow
b_i : light component bottoms flow
b_j : heavy component bottoms flow
W_i: net flow of a component
Φ: roots of underwood equation

DWC:	Divided wall Column
VLE:	Vapor Liquid Equilibrium
LK:	Light Key
HK:	Heavy Key
MK:	Middle Key
MESH:	Mass balance, Equilibrium, Summation and Enthalpy balance.
BASF:	Baden Aniline Soda Factory
BTX	Benzene Toluene Xylene
SC:	Simple Column
PI:	Proportional Integral
PID:	Proportional Integral Derivative
FUG:	Fenske Underwood Gilliland
FTCDC:	Fully Thermally Coupled Distillation Column
MPC:	Model Predictive Control
PR	Peng Robinson
EOS	Equation of State
Viz.	Namely

CHAPTER 1
INTRODUCTION

The process of distillation can be presented as consisting of numerous states of phase equilibrium between flows of liquid and vapor that have different compositions. As a thermal separation method, distillation is one of the most important separation technologies in the chemical industry. Basically, all of the chemicals produced worldwide go through at least one distillation column on their way from crude oil to final product. Considering its many well-known benefits, distillation is and will remain the separation method of choice in the chemical industry with over 40000 columns in operation around the world. Despite the flexibility and the widespread use, one important drawback is the considerable energy requirements, as distillation can generate more than 50% of plant operating costs (Taylor et al., 2003).

The basis of distillation is phase equilibrium, specifically, vapor–liquid (phase) equilibrium (VLE). The process of distillation can be presented as consisting of numerous states of phase equilibrium between flows of liquid and vapor that have different compositions.

1.1. Vapor Pressure

Vapor pressure is a physical property of a pure chemical component. It is the pressure that a pure component exerts at a given temperature when both liquid and vapor phases are present. This dependence is normally a strong one with an exponential increase in vapor pressure with increasing temperature. Equations can be fitted to the experimental vapor pressure data for each component using two, three, or more parameters. For example, the two-parameter version Antoine equation is given as:

$$lnP_j^S = B_j + C_j/T$$

1.2. Binary VLE Phase Diagrams

Two types of vapor–liquid equilibrium diagrams are widely used to represent data for two-component (binary) systems. The first is a “temperature versus x and y” diagram (Txy). The x term represents the liquid composition, usually expressed in terms of mole fraction. The y term represents the vapor composition. The second diagram is a plot of x versus y. These types of diagrams are generated at a constant pressure. Txy diagram, and an xy diagram are convenient

for the analysis of binary distillation systems. The lower curve is the "saturated liquid" line, which gives the mole fraction of benzene in the liquid phase x. The upper curve is the "saturated vapor" line, which gives the mole fraction of benzene in the vapor phase y. In the region between the curves, there are two phases; in the region above the saturated vapor curve, there is only a single superheated" vapor phase; in the region below the saturated liquid curve, there is only a single "sub cooled" liquid phase.

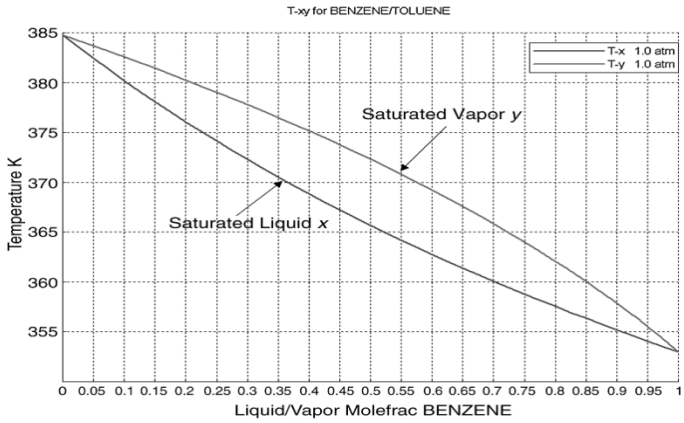


Figure 1.1: Binary VLE phase diagram

1.3. Relative Volatility

One of the most useful ways to represent VLE data is by employing "relative volatility," which is the ratio of the y/x values [vapor mole fraction over (divided by) liquid mole fraction] of two components. For example, the relative volatility of component i with respect to component j is defined in the following equation:

$$\alpha_{ij} \equiv \frac{y_i/x_i}{y_j/x_j}$$

The larger the relative volatility, the easier the separation. Relative volatilities can be applied to both binary and multicomponent systems. In the binary case, the relative volatility a between the light and heavy components can be used to give a simple relationship between the composition of the liquid phase (x is the mole fraction of the light component in the liquid phase) and the composition of the vapor phase (y is the mole fraction of the light component in the vapor phase):

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

1.4. Simple Distillation:

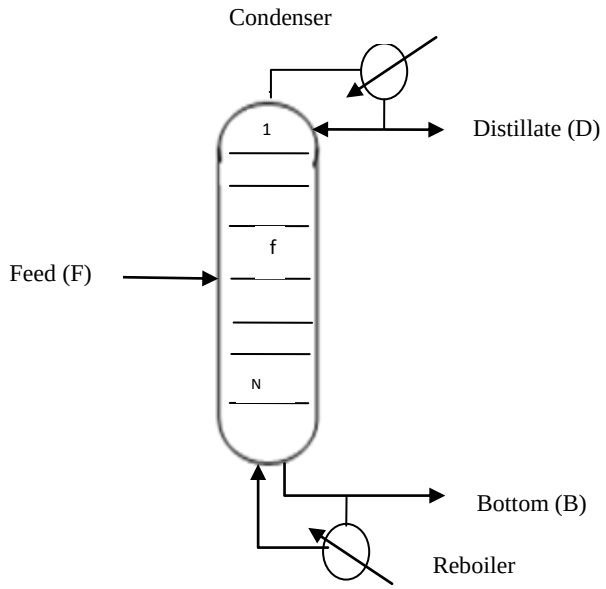


Figure 1.2: An ordinary continuous two-product distillation column

The simple two-product continuous distillation column is shown in Figure 1.2. A binary feed mixture is fed to the feed stage. The column has N equilibrium stages, with the reboiler as stage number N+1. The total molar flow rate of feed is F [mol. /sec] and mole fraction z.

The section above the feed stage is denoted the rectifying section, or just the top section, and the most volatile component is enriched upwards towards the distillate product outlet (D). The stripping section, or the bottom section, is below the feed, in which the least volatile component is enriched towards the bottoms product outlet (B) (The least volatile component is "stripped" out.) Heat is supplied in the reboiler and removed in the condenser, and we do not consider any heat loss along the column. The feed liquid fraction q describes the change in liquid and vapour flow rates at the feed stage:

$$\Delta L_F = qF$$

$$\Delta V_F = (1 - q)F$$

$$q = \frac{h_{V,sat} - h_F}{\Delta H^{vap}} \qquad \text{q is} \begin{cases} > 1 & subcooled\ liquid \\ = 1 & saturated\ liquid \\ 0 < q < 1 & liquid\ and\ vapor \\ = 0 & saturated\ vapor \\ < 0 & superheated\ \ vapor \end{cases}$$

The overall mass balance and component mass balance is given by:

$$F = D + B$$

$$Fz = Dx_D + Bx_B$$

Here z is the mole fraction of light component in the feed, and x_D and x_B are the product compositions. For sharp splits ith $x_D \approx 1$ and $x_B \approx 0$ we then have that D = z × F. In words, we must adjust the product split D/F such that the distillate flow equals the amount of light component in the feed. Any deviation from this value will result in large changes in product composition. McCabe Thiele and Ponchon Savrit methods are used to calculate the reflux ratio and minimum number of stages and the feed stage. With the help of a few of these formulas it is possible to perform a column design in a matter of minutes by hand calculations.

1.5. Multicomponent Distillation

Most of the distillations in the industry involve more than two components. A single distillation column cannot separate more than one component in a reasonably pure form from a multicomponent solution. For a good degree of separation of multicomponent mixture at least a sequence of C-1 distillation columns is needed where C is the number of components. The complexity of multicomponent distillation calculations can be solved by considering a typical problem. The normal procedure is to solve the MESH equations, stage-by-stage, from the top and bottom of the column toward the feed point. For such a calculation to be exact the compositions obtained from both the bottom up and top-down calculations must mesh at the feed point and match the feed composition. But the calculated compositions will depend on the compositions assumed for the top and bottom products at the commencement of the calculations.

1.6. Key Components

We must select the two "key" components between which it is desired to make the separation. The light key will be the component that it is desired to keep out of the bottom product, and the heavy key the component to be kept out of the top product. Specifications will be set on the

maximum concentrations of the keys in the top and bottom products. The "non-key" components that appear in both top and bottom products are known as "distributed" components; and those that are not present, to any significant extent, in one or other product, are known as "non-distributed" components.

1.7. Fenske-Underwood-Gilliland

An approximate method that is widely used for making preliminary designs and simple distillation. The method is commonly referred to as the Fenske-Underwood-Gilliland or FUG method.

1.7.1. Fenske Equation for Minimum Equilibrium Stages

For a specified separation between two key components of a multicomponent mixture, an exact expression is easily developed for the required minimum number of equilibrium stages, which corresponds to total reflux.

$$N_{min} = \frac{Log\{[x_{i,N+1}/x_{i,1}][x_{j,1}/x_{j,N+1}]\}}{Log\ \alpha_{ij}}$$

Equation is extremely useful. It is referred to as the Fenske equation. When i= the light key (LK) and j = the heavy key (HK), the minimum number of equilibrium stages is influenced by the non-key components only by their effect (if any) on the value of the relative volatility between the key components. Equation above permits a rapid estimation of minimum equilibrium stages. A more convenient form of is obtained by replacing the product of the mole-fraction ratios by the equivalent product of mole-distribution ratios in terms of component distillate and bottoms flow rates d and b, respect and by replacing the relative volatility by a geometric mean of the top-stage and bottom-stage values. Thus,

$$N_{min} = \frac{Log\{[d_i/d_j][b_j/b_i]\}}{Log\ \alpha_m}$$

Where the mean relative volatility is approximated by:

$$\alpha_m = [(\alpha_{ij})_N(\alpha_{ij})_1]^{1/2}$$

The minimum number of equilibrium stages depends on the degree of separation of the two key components and their relative volatility, but is independent of feed-phase condition.

1.7.2. Gilliland Correlation for Actual Reflux Ratio and Theoretical Stages

To achieve a specified separation between two key components, the reflux ratio and the number of theoretical stages must be greater than their minimum values. The actual reflux ratio is generally established by economic considerations at some multiple of minimum reflux.

$$Y = \frac{N-N_{min}}{N+1} = 1 - \exp\left[\left(\frac{1+54.4X}{11+117.2X}\right)\left(\frac{X-1}{X^{0.5}}\right)\right]$$

$$\text{Where, } X = \frac{R-R_{min}}{R+1}$$

1.7.3. Underwood Equations

Consider a two-product distillation column with a multicomponent feed (F) with liquid fraction q and composition vector z of N components. The defining equations for the Underwood roots (ϕ) in the top and (α_i) in the bottom are:

$$Top: V_T = \sum_{i=1}^{N} \frac{\alpha_i W_{i,T}}{\alpha_i - \phi}$$

$$Bottom: V_{\boldsymbol{B}} = \sum_{i=1}^{N} \frac{\alpha_i W_{i,B}}{\alpha_i - \psi}$$

$$V_T - V_B = \sum_{i=1}^{N} \frac{\alpha_i (W_{i,T} - W_{i,B})}{\alpha_i - \theta} = \sum_{i=1}^{N} \frac{\alpha_i Z_i F}{\alpha_i - \theta} = (1-q)F$$

Where W_i is the net flow of a component. There will be N solutions for each root, and the solution sets from the top and bottom equations are generally different. However, Underwood showed that the roots obey$\alpha_i \geq \phi_i \geq \psi_{i+1} \geq \alpha_{i+1}$. Furthermore, with an infinite number of stages, at minimum vapor flow, one or more pairs of roots (ϕ_i, ψ_{i+1}) in the top and bottom coincide to a set of common roots (θ_i). The set of N - 1 possible common roots are obtained by setting $\phi_i, \psi_{i+1}, \theta_i$ and subtracting the two defining equations above. This gives the feed equation where the set of common roots depends only on the feed properties R, z, and q.

1.8 Conventional Distillation Sequences

Considering a mixture of A, B & C, here A is most volatile component and B is the least volatile component. For a ternary separation two columns are needed for the satisfactory separation of the components into pure products. Each of these columns has a rectifying and a stripping section. So the minimum number of column sections is four to receive pure products. If one

reboiler for each stripping section and one condenser for each rectifying section are used, than this leads to the conventional distillation sequences: direct and indirect split, which are shown in with in total four reboilers and condensers. But as stated above these configurations are not possible to perform reversible splits and will therefore in general need more energy for the separation than reversible splits. Figure 1.3 shows the conventional distillation sequences the indirect and the direct sequence

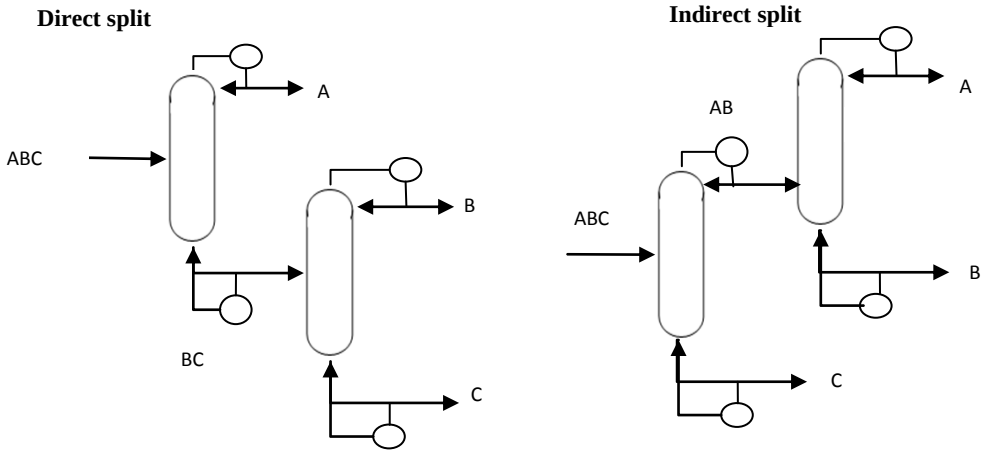


Figure 1.3: Conventional Distillation Sequences

1.9 Thermally Coupled Distillation Column

A further capital saving benefit can be arranged, where appropriate, by removing condenser and the reboiler of the prefractionator column. This leads to a configuration shown schematically in Fig.1.4 and is generally known as "Petlyuk column". In fact, omitted condenser and reboiler are effectively replaced by thermal (heat) coupling of prefractionator column with the main column, with the necessary condenser and reboiler being attached to the main column. Therefore this configuration is generally known as "fully thermally (heat) coupled column". Its salient feature lies in the use of the pre-fractionator column from which a non-sharp split of light (A), medium (B) and heavy (C) components into two mixtures occurs. The top product of the pre-fractionator contains A and B and the bottom product contains B and C. These mixtures are introduced into the main column by the thermal coupling arrangement of the top and the bottom of the pre-fractionator. In the main column, these components are separated into three distinct products. Most of the energy savings in the Petlyuk column arrangement are attributed to the pre-fractionator. A major source of separation inefficiency in conventional multicomponent

distillation is the re-mixing effects that occur. A significant reduction in the re-mixing inefficiency is provided by a non-sharp split in the pre-fractionator.

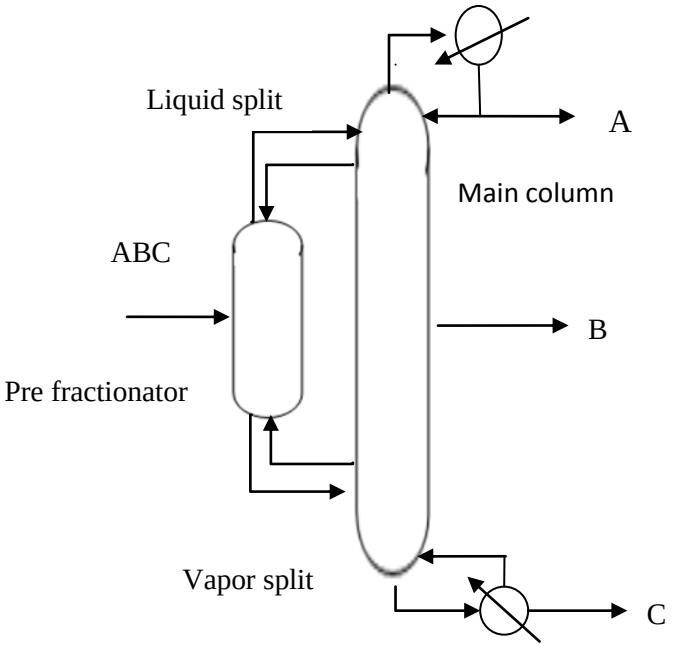


Figure 1.4: Petlyuk column

1.10 Divided Wall Column

Conventionally, a ternary mixture can be separated via a direct sequence (most volatile component is separated first), indirect sequence (heaviest component is separated first), or distributed sequence (mid split) consisting of two to three distillation columns. This separation sequence evolved to the Petlyuk column configuration consisting of two fully thermally coupled distillation columns. Eventually, this led to the concept known today as dividing-wall column (DWC) that integrates in fact the two columns of a Petlyuk system into one column shell. Figure 1.3 illustrates the most important ternary separation alternatives.

The name of DWC (dividing-wall column or divided wall-column) is given because the middle part of the column is split into two sections by a wall, as illustrated in Figure 1.5 When a multi-component feed is introduced to the pre-fractionator side of the DWC, the low- (LK) and high-boiling point components (HK) are separated in the pre-fractionator while the middle boiling component (MK) distributes to the top and the bottom of the wall along with LK and HK respectively. Further separation of LK and MK occurs in the upper section of the main column

while the separation of HK and MK occurs in the lower section of the main column. As the composition of the MK at the top and the bottom of both sides of the dividing wall have to be matched, concentration of the MK reaches a peak value in the middle section on the other side of the wall. A high purity MK can then be withdrawn from the middle section of the main column, as a side draw. Sharp split between LK and HK achieved in the pre-fractionator effectively reduces the contamination of MK drawn at the other side of the wall. This is simply because neither the LK can pass to the bottom section of main column nor the HK can pass to the upper section of the main column provided there is no azeotrope present in the mixtures hence, the MK can be withdrawn at its maximum concentration from the other side of the wall. Simultaneously, the problem of re-mixing in the conventional columns when feedstock contains more than two components is avoided (Triantafyllou and Smith, 1992).

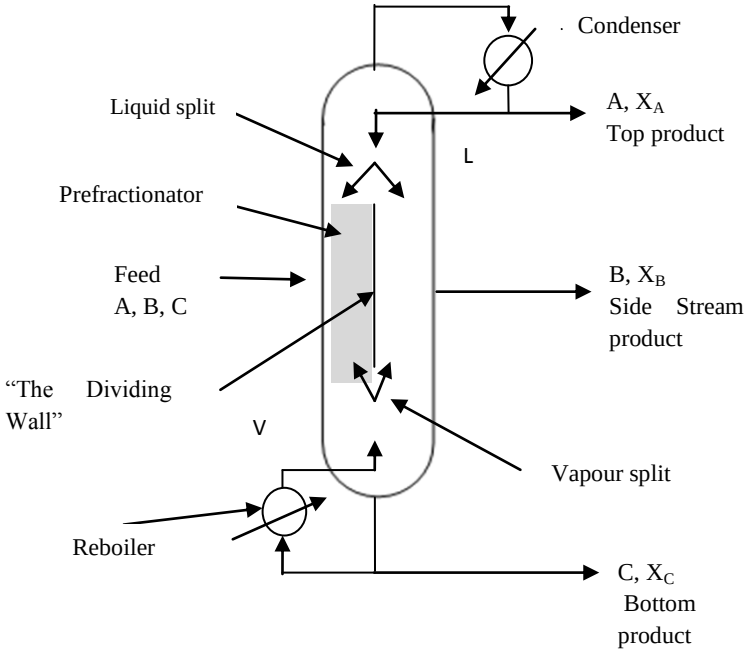


Figure 1.5: A Divided Wall Column

In addition, the distribution of MK between the top and the bottom of the pre-fractionator provides greater freedom for the selection of proper feed stage to ensure better matching between the feed stream composition and the composition of the tray. This leads to significant reduction in the mixing losses at the feed tray. The fully thermally coupled column or the Petlyuk column (Fig. 1.5) which has been known for around 50 years can also save the energy of about 30%

compared to the conventional sequences (Petlyuk et al., 1987). Dividing wall column (DWC) reduces investment cost by 25%, operating cost by 35% Schultz et al (2002), and space requirements by 40%, as compared to the conventional column system. The construction of the Petlyuk column maybe carried out in a single shell with a dividing wall installed to separate the pre-fractionation from the main column section. As a result, the dividing-wall column (DWC, Fig. 1.5) can save the capital investment by around 30% Triantafyllou and Smith (1992).

The world's first DWC was established by BASF in 1985 (Parkinson, 2007). Dividing wall columns gained increasing application in the last years. More than 90 applications in production scale are known (Asprion and Kaibel, 2010). Around 70 packed DWCs were reported, some of notable dimensions (diameters above 4 m and heights up to 80 m), in operation in BASF plants worldwide. Internals for nearly all of these columns have been delivered by J. Montz GmbH, and the necessary process and mechanical design knowhow was developed in close cooperation of BASF and Montz. Practical implementation at BASF has been accompanied by two German and subsequently European patents issued in 1984 to G. Kaibel of BASF AG (Dejanovic et al., 2010).

DWC is very appealing to the chemical industries with BASF, UOP, Linde AG and Uhde as the leading companies because it can separate three or more components in a single tower, thereby eliminating the need for a second unit, hence saving the cost of building two columns and cutting operating costs.

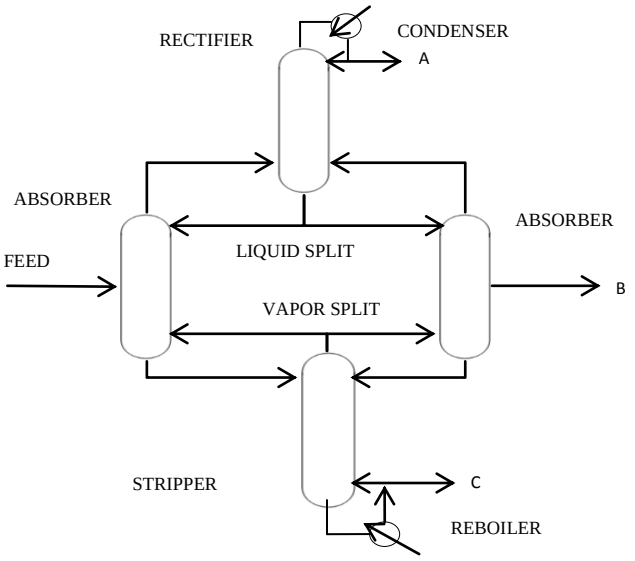


Figure 1.6: Struture used to represent DWC

Fig. 1.6 shows the structure used in the analysis of divided wall column in the present study, (Ling and Luyben, 2009). The four columns are one rectifier, one splitter and two absorbers. These models are arranged as shown in Fig. 1.6.

Compared to classic distillation design arrangements, DWC offers the following benefits:

1. High purity for all three or more product streams reached in only one column.
2. High thermodynamic efficiency due to reduced remixing effects.
3. Lower capital investment due to the integrated design.
4. Lower energy consumption compared to conventional direct, indirect and distributed separation sequences.
5. Small footprint due to the reduced number of equipment units compared to conventional separation configurations.

CHAPTER 2
LITERATURE REVIEW

Several studies have indicated that DWC can save up to 30% on energy consumption with respect to conventional direct and indirect distillation sequences (Glinos and Malone, 1988; Triantafyllou and Smith, 1992; Wolff and Skogestad, 1995).

Triantafyllou and Smith (1992) gave a first design oriented method for a separation of ternary mixture in DWC based on Fenske-Underwood-Gilliland-Kirkbride model (FUGK) to establish the minimum number of equilibrium stages (Fenske), minimum reflux (Underwood), stage requirement at the chosen reflux ratio (Gilliland) and the feed stage location (Kirkbride equation) for a given separation. Basic assumptions of this model were constant relative volatility and constant molar flows.

Wolff et al. (1995) performed control studies on the Petyluk configuration using a three point and four point composition control. For the three point composition control, they set up a control configuration which maintained the composition of the three main products of the column. Using one of the possible control schemes, they were able to achieve satisfactory control performance, given feed flow-rate and composition and set point disturbances. For the four point composition control, they used the internal liquid split between the pre-fractionator and the main column to control the impurity ratio in the side draw as an additional control loop. They learned that a problem could occur within a range of the internal liquid splits whereby the product specifications cannot be achieved. A similar result was observed when the vapour split was used in place of the liquid split.

Hernandez and Jimenez (1996) gave rigorous dynamic model for the design of both direct and indirect thermally coupled distillation sequences for ternary system for minimizing the total heat duty.

Halvorsen and Skogestad (1997) showed how liquid and vapour splits were related to vapour boil up rate in a Petlyuk column and suggested to use the liquid split for control to minimize the energy input to the column. They suggested some control variables and described the ideal self-

optimizing control properties of such measurements. Temperature differences in the column were one of the suggested measurements, but no dynamic simulation results were presented.

The complexity of DWC operation and control was assessed by (Mutalib and Smith, 1998). They investigated the impact of liquid and vapour split ratio on the operation and control of a DWC, based on dynamic simulation. A pilot plant study for the operation and control of a DWC was conducted by (Mutalib et al., 1998) by using temperature control. Pilot plant and simulation studies using temperature controls showed that there was an offset in one of the product purities.

Agrawal and Fidkowski (1998) showed that a DWC configuration was favorable only in certain operating region. Abdul Mutalib and Smith (1998) and Abdul Mutalib et al. (1998) investigated the effect of liquid and vapor splits on the design and control of DWC. They found that design for liquid and vapor splits should be based on the highest product specifications and two proposed composition control schemes are satisfactory.

Mizsey et al. (1998) studied the Petlyuk column choosing control the three product compositions while keeping the liquid split fixed.

Dunnebier and Pantelides (1999) suggested that DWC have not widely used in industrial practice largely due to controllability concerns. Hernandez and Jimenez (1999) compared DWC with controllability of different distillation arrangements. They found that DWC was the most difficult to control. Amminudin et al. (2001) developed a semi-rigorous method based on the concept of equilibrium stage composition for the initial design of a DWC, which can be employed any established non-linear optimization solver. Dünnebier and Pantelides (1999) proposed a rigorous design method based on detailed column superstructures for a given separation task, followed by mathematical optimization.

Muralikrishna et al. (2002), was used to get the input data necessary to initialize the rigorous simulations. The results obtained for the hybrid structures were compared with the performance of the best SC sequence from which the energy and capital cost savings were evaluated. The Petlyuk and the DWC structures were considered independently for the capital cost evaluation to select the most economic configuration. Significant energy reduction was achieved with DWC schemes, while the saving in the capital costs was lower than the 30% value reported in most of the specialized literature.

Adrian et al., (2002) compared using three single temperature loops (PI-controllers) against a (multivariable) model predictive controller (MPC). They used the reflux (L) to control a

temperature in the top of the pre-fractionator, the side-stream rate (S) to control a temperature in the bottom section and the liquid split to control a temperature in the main column above the side draw. They concluded that MPC showed superior control behavior to that of the decentralized feedback loops. However, it should be noted that the vapour boil up V was kept fixed during the PI experiments, while it was used as an extra input for the MPC experiment.

Using the same controllability indexes as those of Hernandez and Jimenez (1999), Serra et al. (2003) compared the controllability of different multi-component distillation arrangements and discussed the operation conditions that favor controllability for the DWC.

Adrian et al. (2004) compared model predictive control (MPC) with PI control for an experimental DWC. They found that MPC has superior control behavior, better constraint handling, and considerable economic benefits; but required substantially more efforts of modeling and parameter tuning.

Halvorsen and Skogestad (2004) studied the energy consumption of a DWC using shortcut analysis. They found that the two additional degrees of freedom: liquid and vapor split ratios are important to the energy efficiency.

Kim (2005) proposed a structural design procedure for FTCDC using a semi-rigorous model and tested on three separation systems, viz. isomers of butanol, BTX and hexane/2-methyl hexane/heptane mixtures having different feed compositions. The design procedure employed material balances and equilibrium calculated using UNIQUAC activity model and the Peng–Robinson equation of state for the computation of tray compositions. The structural information was utilized in HYSYS simulations to find the operating variables that would meet a given set of product specifications. The outcome of the structural design was used as initial estimate for the rigorous simulation.

Kim (2006 a, b) also suggested a new system of a FTCDC, and inspected its performance on two industrial processes. The system had an extra column called post-fractionator, attached to the main column of an original FTCDC. The structure of FTCDC system was implemented for the fractionation process of a naphtha reforming plant for BTX separation and the gas concentration process to give gas products from a gas mixture taken out from crude distillation, naphtha reformation and naphtha-cracking processes in a refinery. The result of the performance analysis using HYSIS showed a 29 % energy saving with fractionation process and a 7 % saving with gas

concentration process over the original FTCDC. In addition, he also discussed the new column construction, such as arrangement of distillation column sections and divided wall construction.

Rangaiah et.al (2009) presented simulation and optimization results of DWCs for six diverse feed mixtures using HYSYS, the outcomes lead to useful recommendations for the design of DWCs. The detailed design and optimization procedures for a ternary system Benzene- Toluene-p-Xylene (BTX) system. For the initialization of rigorous simulation and design of DWC three-column shortcut simulation was carried out it provided reasonable estimates.

Rong and Turunen (2009) studied DWC configurations for the separation of a four components mixture with five different feed compositions. The best Simple Column (SC) configuration was chosen as the basis for the comparison with the new configurations obtained by introducing a Petlyuk/DWC structure. The most promising cases correspond to Petlyuk/DWC fed with equimolar of equal excess of lightest and middle component mixtures.

Ling and Luyben (2009) discussed a new control structure for DWC that was capable of simultaneously controlling product compositions and minimizing energy consumption in a practical way. The aim was to control p-xylene composition at the top of the prefractionator side of the wall by manipulating the liquid split. Steady-state relationships show that maintaining this composition produces energy consumptions that are very close to the minimum values as feed compositions change.

Ling and Luyben (2010) studied two types of temperature control structures. In the first, the four manipulated variables were adjusted using three temperatures located in the main column and one temperature on the prefractionator side of the wall. This structure was able to handle feed flow rate disturbances, but product purities started deviating significantly from their desired values for feed composition changes greater than about 10%. In the second control structure, four differential temperature control loops were used. The performance was found to be improved and disturbances of 20% in feed composition were well handled with only small deviations in product purities. This structure also handled large changes in column operating pressure.

Dejanovi´c et al. (2010) provided a complete outline of the work done on the research and implementation of DWCs based on published papers and patent literature, from early ideas on thermal coupling of distillation columns to practical issues that need to be solved for their successful implementation. Approaches to short-cut and rigorous simulation, optimization, and

control were highlighted, with particular focus on column internals and dimensioning. A survey of relevant patents was included providing information on equipment innovations and application areas of industrial interest.

Asprion and Kaibel (2010) studied the recent advances in the field and the fundamentals of DWC, such as the application of DWC to more than three components, its application in reactive distillation processes such as the ester hydrolysis of methyl acetate for methanol/methyl acetate mixtures, control of dividing wall columns, start-up procedure dividing wall columns for batch distillation, use of exergy analysis for dividing wall column and optimization of petlyuk arrangements.

Diggelen et al. (2010) compared a number of different decentralized control configurations and more advanced multivariable controllers on a dynamic model of a Petlyuk column. The objective was to control the product compositions at their set points. In the case for the decentralized configurations three composition loops were closed, while the liquid split was kept constant. They found that while the decentralized PI controllers work, disturbances were controlled faster using MIMO (multi-input, multi-output) controllers.

Yildirim et al. (2011) gave an overview of the some important DWC control structures. The dynamic optimization. Kiss and Rewagad (2011) proposed DWC control structures based on PID controllers in a multi-loop framework , the proposed structure was able to simultaneously control the products compositions and minimize the energy requirements. was based on a simple strategy, which was to control the heavy component composition at the top of the pre-fractionator side of the DWC by manipulating the liquid split ratio. The steady-state relationships showed that maintaining or minimizing this composition lead to energy requirements that were near or at the minimum values as feed composition change.

Ling et al. (2011) explored a new control structure for the separation of benzene, toluene, and o-xylene by controlling the remixing of the intermediate at the top trays in the prefractionator section. They found that the divided-wall column work very close to the optimal conditions when the remixing of toluene is avoided. The remixing of toluene was studied at steady state first. After that they employed a remixing control structure with the remixing control loop and three composition control loops. By avoiding the remixing of toluene at the top of the prefractionator minimized energy consumption was achieved. Disturbances in feed flow rate and feed compositions were used to demonstrate the effectiveness of the proposed control structure.

Kiss and Rewagad (2012) studied the advanced control strategy based on MPC to perform dynamic optimization of a DWC. The dynamic model of the DWC used in their study was not a reduced one but a full-size nonlinear model that was representative of industrial applications. The quality of the linearized model used for the predictions inside MPC was derived from and tested against the nonlinear model. The variables were selected to achieve the aim of regulatory and inventory control in the column, at the same time minimizing the energy requirements in a very practical way.

Sangal et al. (2012a) carried out the degrees of freedom analysis of a divided wall distillation column for steady state by using detailed mathematical model, which contains the MESHD equations (conventional MESH equation plus the pressure drop equation). According to them, pressure difference played an important role in a divided wall distillation column in deciding vapour and liquid flow rates across trays in the divided section. It was observed that for a given divided wall distillation column or Petlyuk column operating under steady state conditions with known feed and condenser pressure, the degrees of freedom was four. This was one higher than that for a conventional distillation column with three product streams (distillate, bottoms and the intermediate product). No extra degree of freedom was left to specify vapour split ratio if this extra degrees of freedom was used to specify liquid split.

Sangal et al. (2012b) optimized different structural and process parameters of a divided wall column (DWC) for the energy efficiency. The operation and optimal design of DWC is a non-linear problem and involves a number of variables. Rigorous simulation of a DWC was carried out using Multifrac model of ASPEN Plus software. For the optimization of the parameters and to evaluate the effects of these parameters and their interactions on the energy efficiency of a DWC, Box–Behnken design (BBD) under response surface methodology (RSM) was used. As compared to the effect of structural variables, the process variables were found to have significant effect on the energy efficiency of a DWC and the predictions from the BBD optimization agreed well with the results of the rigorous simulation.

Sangal et al. (2012c) carried out a simulation of a divided wall column (DWC) for the separation of C4-C6 normal ternary paraffin mixture to study the product quality and energy efficiency as a function of reflux rate, liquid spilt and vapour split. Rigorous simulation of the DWC was carried out using Multifrac model of ASPEN Plus software. To evaluate the effects and interaction of the process parameters such as reflux rate (r), liquid split (l) and vapour split (v). Box–Behnken

design (BBD) was used for the optimization of parameters. It was found that for the optimization of DWC by this method the number of simulation runs reduced significantly.

Sangal et al. (2012d) carried out a theoretical investigation to find out a relation between natural or feasible vapour split ratio as a function of reflux ratio and the liquid split ratio for a DWC. The MultiFrac model of ASPEN PLUS was used for simulation of the DWC for the fractionation of a ternary BTX mixture. They showed that the consideration of pressure drop during distillation column simulation was necessary and that tray hydraulics played an important role on the column performance. In case of interlinked columns such as a DWC, consideration of pressure drop becomes necessary as vapour split ratio cannot be maintained at a desired value and it is completely determined by the vapour phase hydrodynamics of the column.

CHAPTER 3

SIMULATION OF DWC

Simulation of a DWC is a challenging task, as it involves numbers of variables. Aspen Plus and Aspen Dynamics are powerful tools used, in order to build the shortcut and rigorous steady-state simulations. In order to simulate a DWC initial estimates of some parameters are required, for estimation of these parameters we need to carry out shortcut simulation of DWC.

3.1 Shortcut Simulation of DWC

Shortcut simulation was done using DSTWU model. In shortcut simulation three DSTWU blocks were used to represent the DWC structure. DSTWU performs Winn-Underwood-Gilliland shortcut design calculations for a single-feed, two-product distillation column, with a partial or total condenser. For the specified recovery of the light and heavy key components, DSTWU estimates the minimum for either:

- Reflux ratio
- Number of theoretical stages

DSTWU also estimates:

- Optimum feed stage location
- Condenser and reboiler duties

Figure 3.1 shows three DSTWU models used for shortcut simulation.

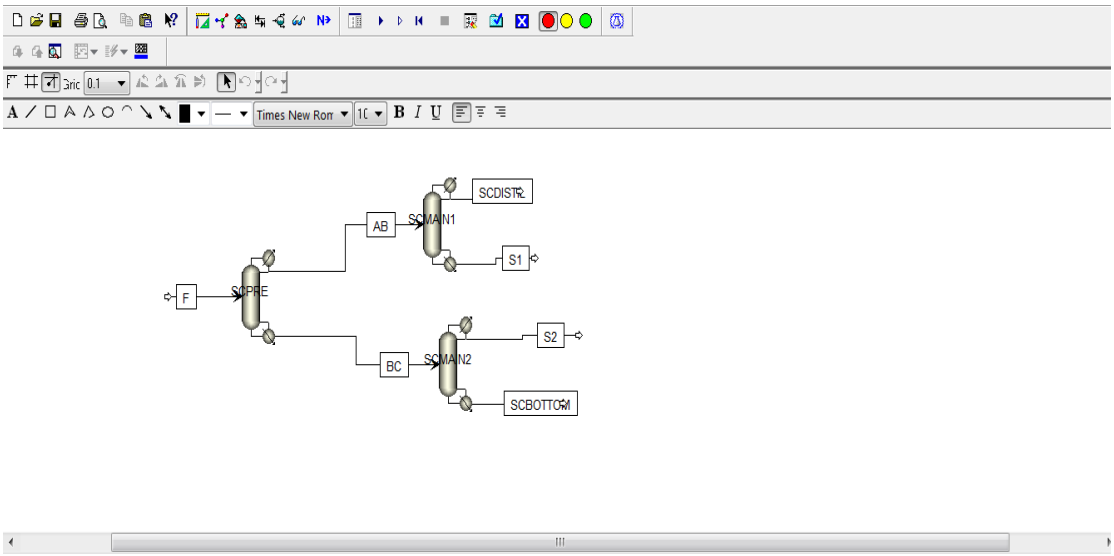


Figure 3.1.: Flow sheet of shortcut simulation

The simulation gave following results:

Stages above pre fractionator	11
Reflux ratio	4
Number of stages in pre fractionator	26
Feed stage	13
Stages below pre fractionator	12

3.2 Rigorous Simulation Using Radfrac (Steady State Study of Process)

RadFrac is a rigorous model for simulating all types of multistage vapor-liquid fractionation operations. These operations include:

- Ordinary distillation.
- Absorption.
- Stripping.
- Extractive and azeotropic distillation.

The steady-state Radfrac model in Aspen Plus consisted of four column sections: one stripper, two parallel absorbers, and a rectifier as shown in figure 3.2. In reality, there is only one column, but these four "fictitious" vessels are used in the simulation to model the real physical equipment (ling and luyben, 2010). The blocks used in the structure are named as the stripper is named "STRIPPER", rectifier is named as "RECTIFR", absorber block used on the prefractionator was named "ABSRBR1", and another absorber block on the side stream side was named as "ABSRBR2". Two splitters were used in the model one was connected in the liquid outlet stream of the block "RECTIFR" it was named "LIQSPL" and the other was in the vapor outlet at top of the block "STRIPPER" named as "VAPSPL", these two blocks represent the liquid split and the vapor split respectively. Feed input is in "ABSRBR1" and the side product is withdrawn from "ABSRBR2". The top and bottom products are withdrawn from top of "ABSRBR1" and bottom of "ABSRBR2" respectively.

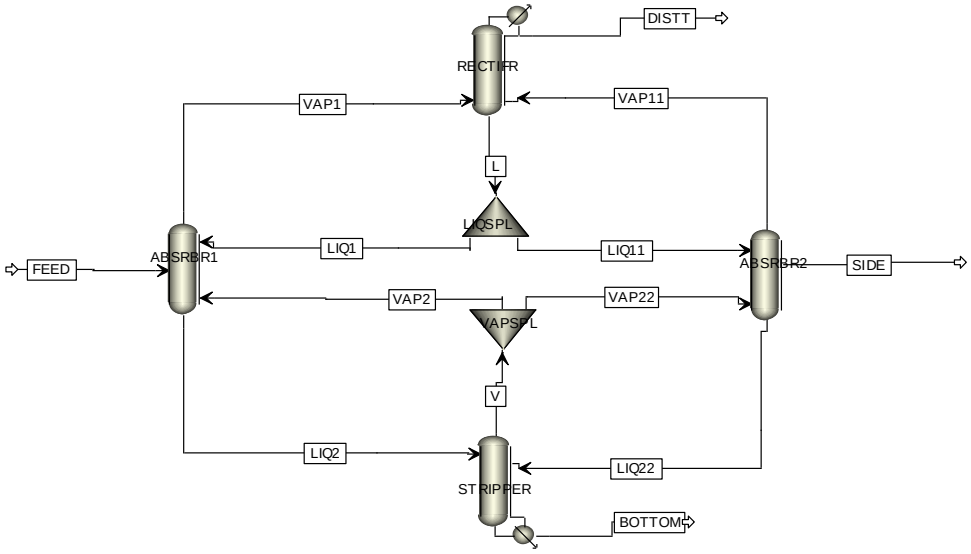


Figure 3.2: Steady state flow sheet of DWC

The feed conditions for the steady state are same as the shortcut simulation only the column specifications change. The specifications for the feed, feed conditions, product, and other required operating conditions are given in Table 3.1.

Table 3.1: Specifications for the steady state simulation.

Components	Mole fraction	Feed Conditions	Product specifications	Operating conditions	Fluid package
Benzene Toluene p-Xylene	0.3 0.3 0.4	3600Kmol/hr 1 atm. Saturated liquid	D=98% S=98% B=98%	Total condenser=0.37 atm.	PR

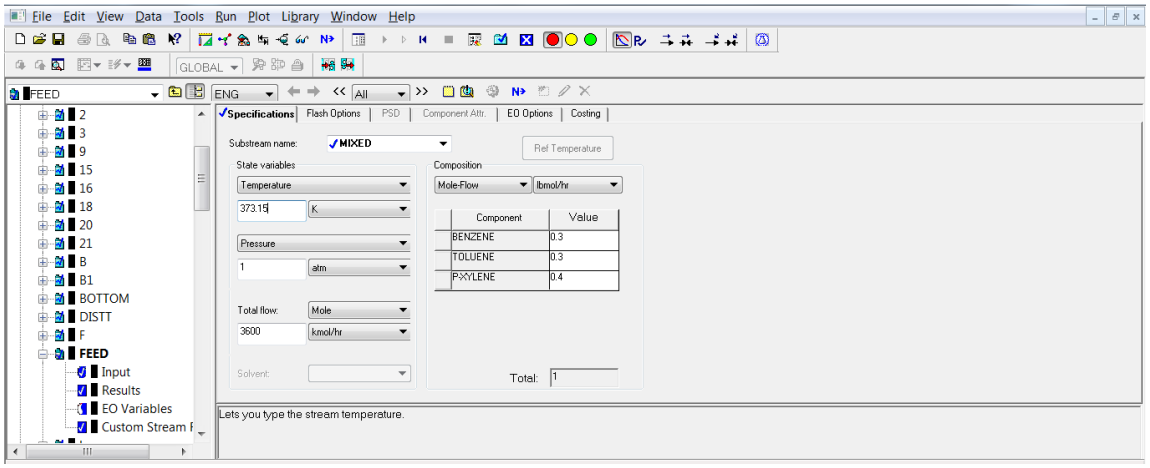


Figure 3.3: Specification sheet for feed conditions

The data for the number of stages were entered in the specification sheet for the block ABSRBR1 as shown in Fig. 3.4. the type of condenser and reboiler were entered as none as the there are no condenser or reboiler on the absorber model.

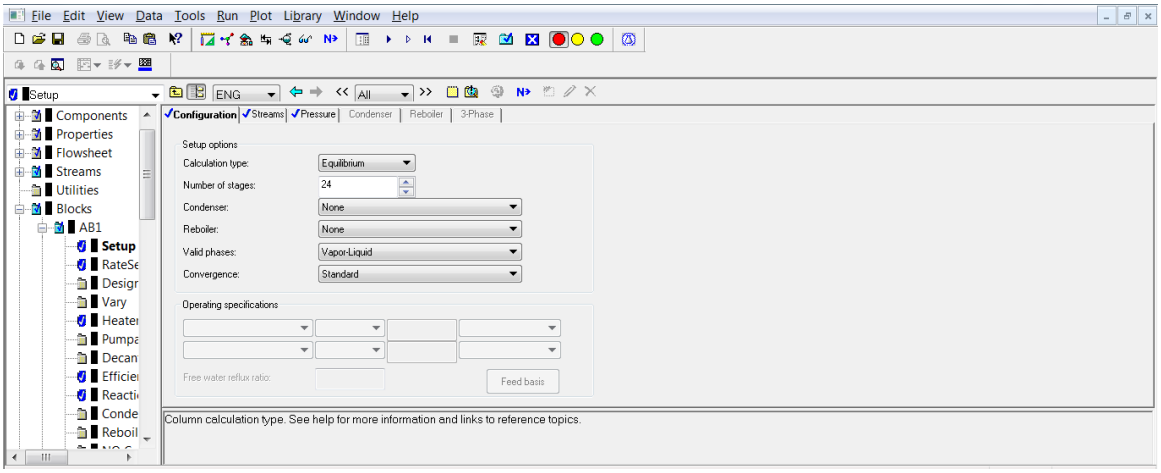


Figure 3.4: Specification sheet for block ABSRBR1 (setup)

The data for the stage number of the feed stream and the phases of product stream was entered as shown in Fig. 3.5.

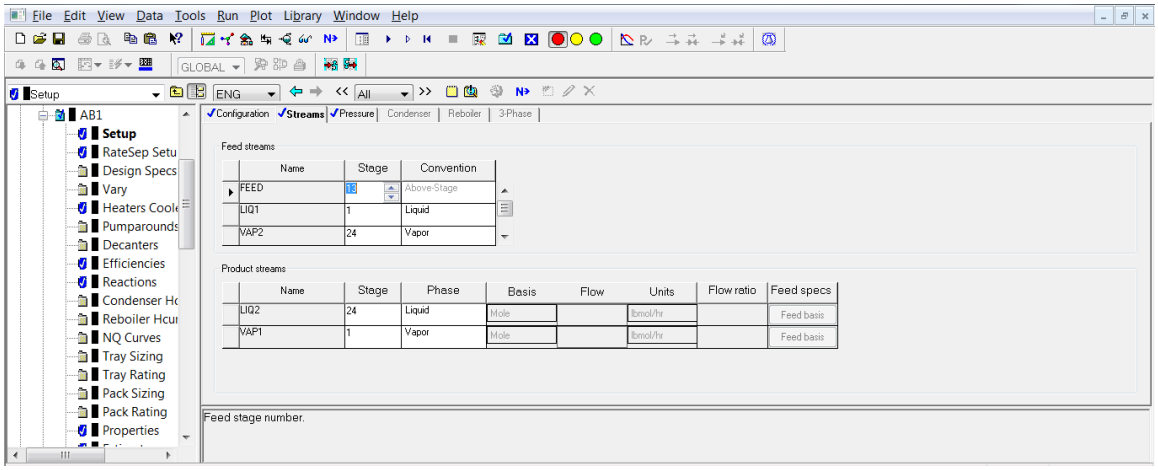


Figure 3.5: specification sheet for block ABSRBR1 (streams)

The number of stages for the block ABSRBR2 were specified as shown in Fig. 3.6.

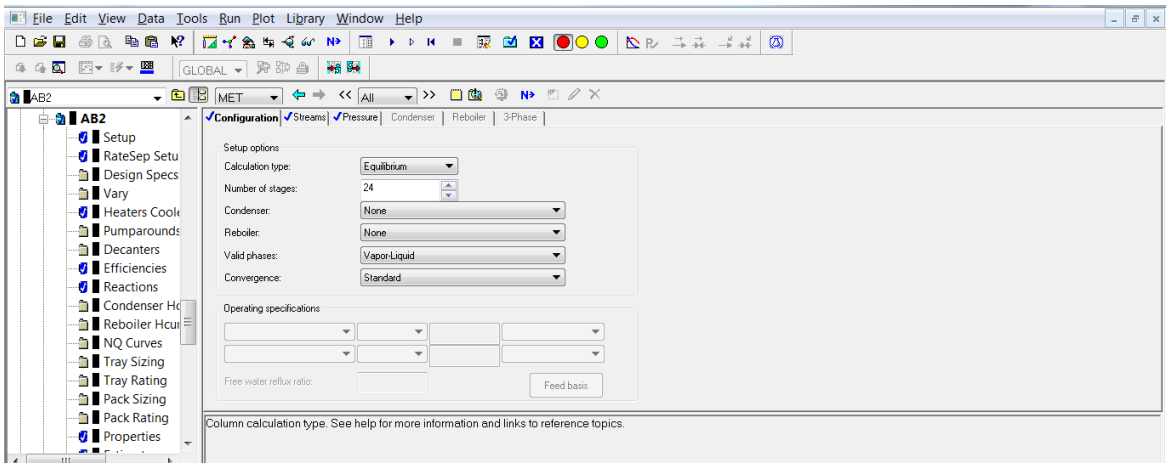


Figure 3.6: Specification sheet for block ABSRBR2 (SETUP)

The input data for the streams connected to the block was specified as shown in Fig. 3.7.

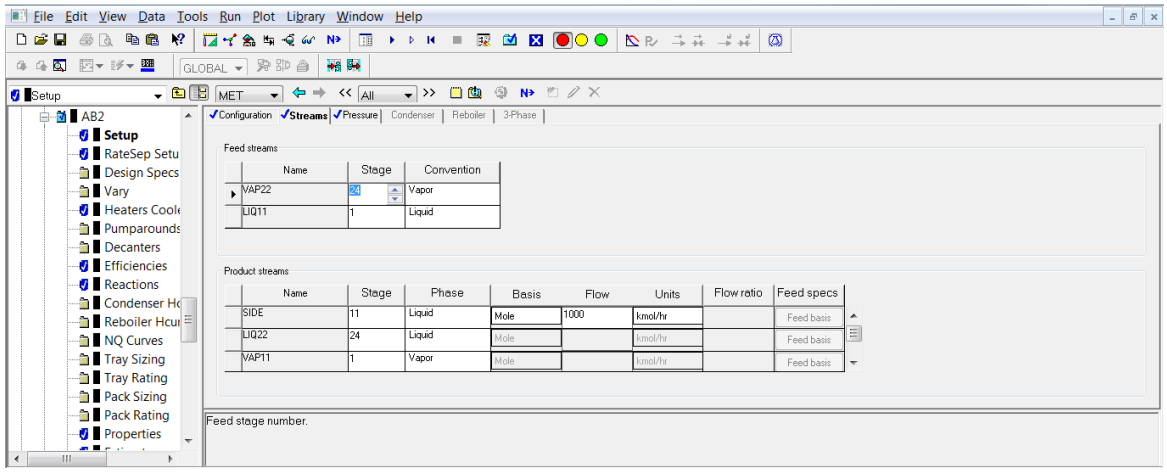


Figure 3.7: specification sheet for block ABSRBR2 (STREAMS)

The split fraction was specified for the blocks LIQSPL and VAPSPL as shown in Fig 3.8 and 3.9. The split is defined as the ratio between the flow on the product side to the flow on the feed side of the dividing wall.

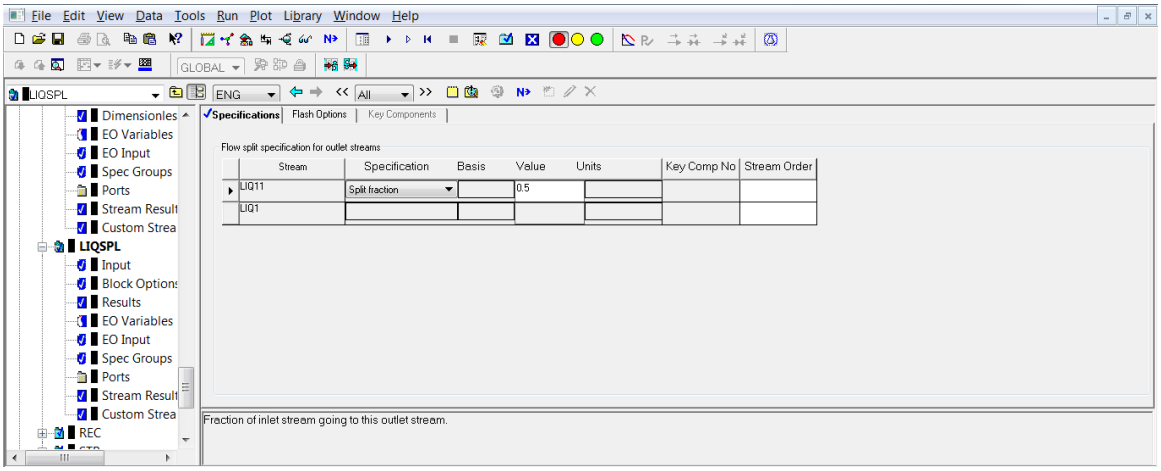


Figure 3.8: specification sheet for block LIQSPL

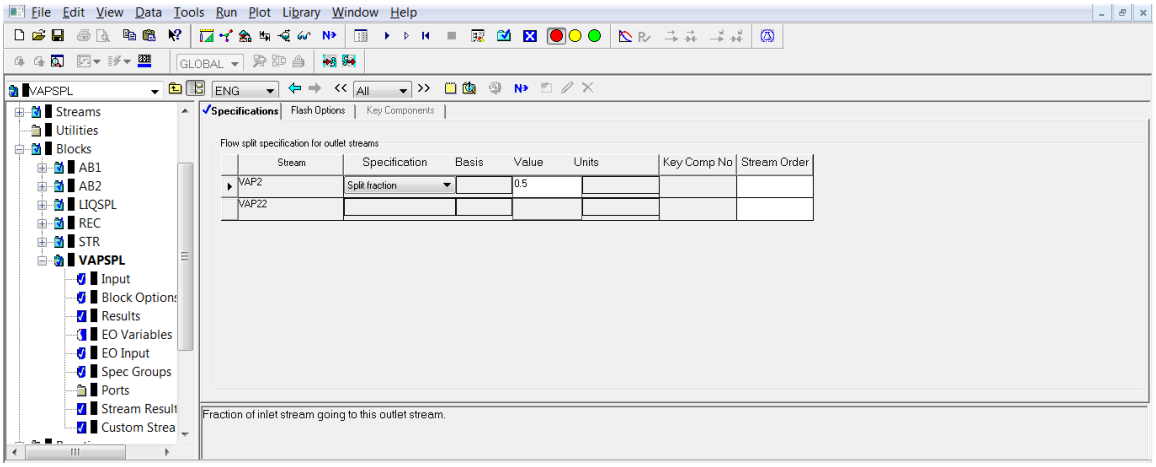


Figure 3.9: specification sheet for block VAPSPL

The specifications for the block RECTIFR for the type of condenser, number of stages reflux ratio (Fig. 3.10), the streams connected to the block (Fig. 3.11), and the pressure within the column (Fig. 3.12) was entered in and the condenser is specified as "Total" and reboiler as "none" as shown in Fig. 3.10. Similarly, the same input sheets required to be filled for the block STRIPPER, here the type of condenser was specified as none and the bottoms rate was provided for the block as shown in Fig. 3.13. the data for the streams was entered in the form as shown in Fig. 3.14.

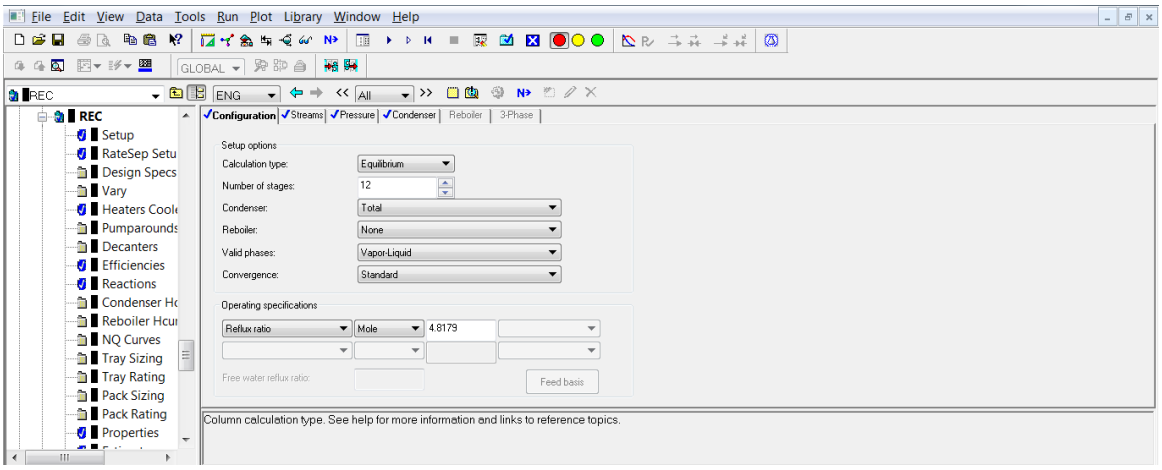


Figure 3.10: specification sheet for block RECTIFR (SETUP)

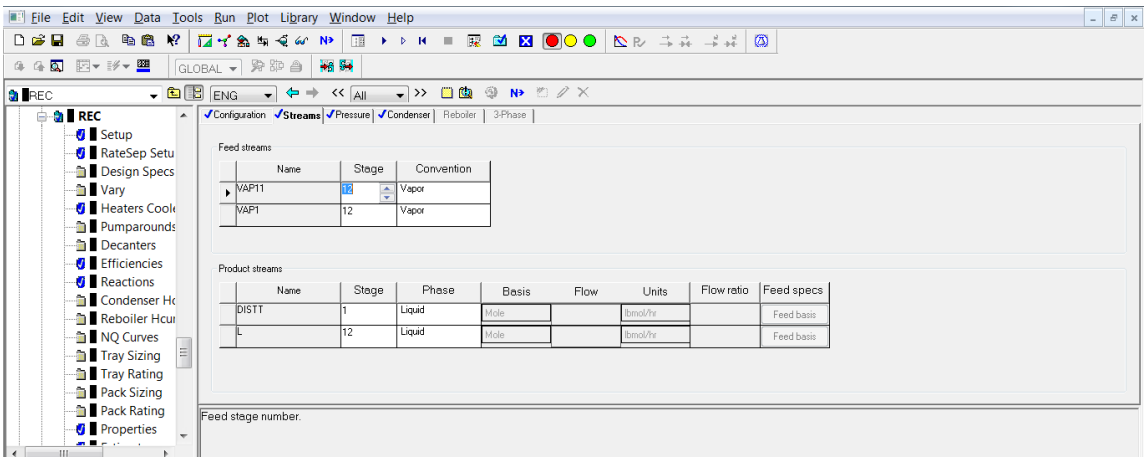


Figure 3.11: specification sheet for block RECTIFR (STREAMS)

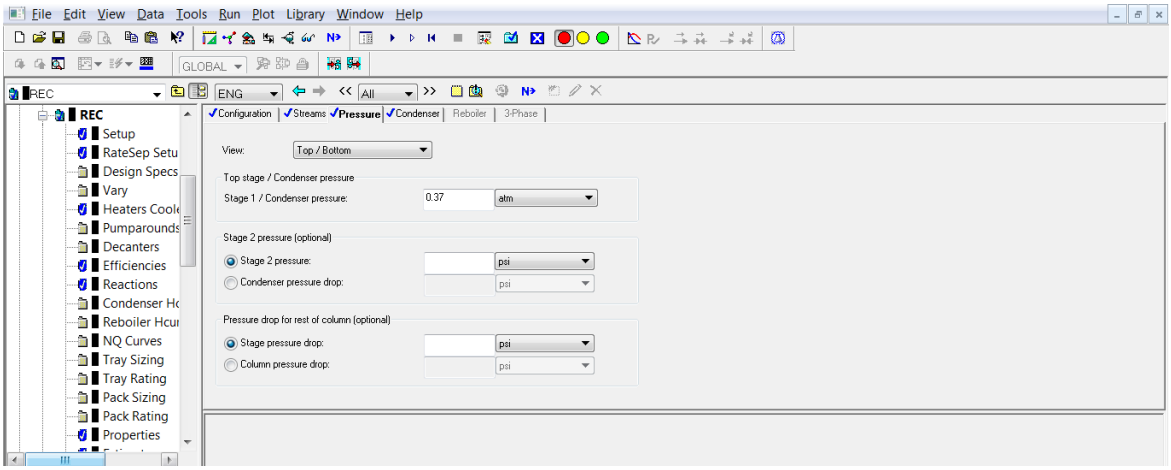


Figure 3.12: specification sheet for block RECTIFR (PRESSURE)

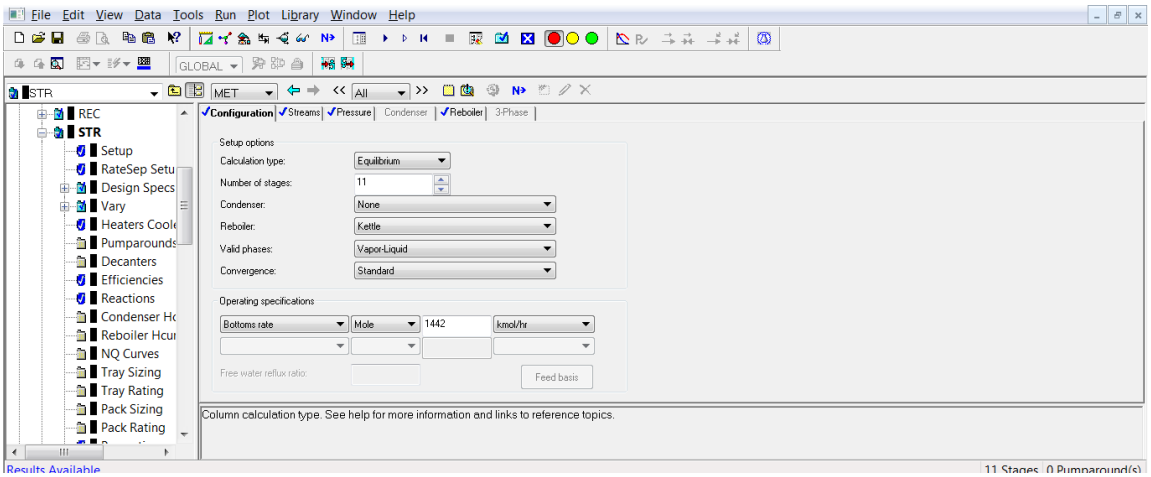


Figure 3.13: specification sheet for block STRIPPER (SETUP

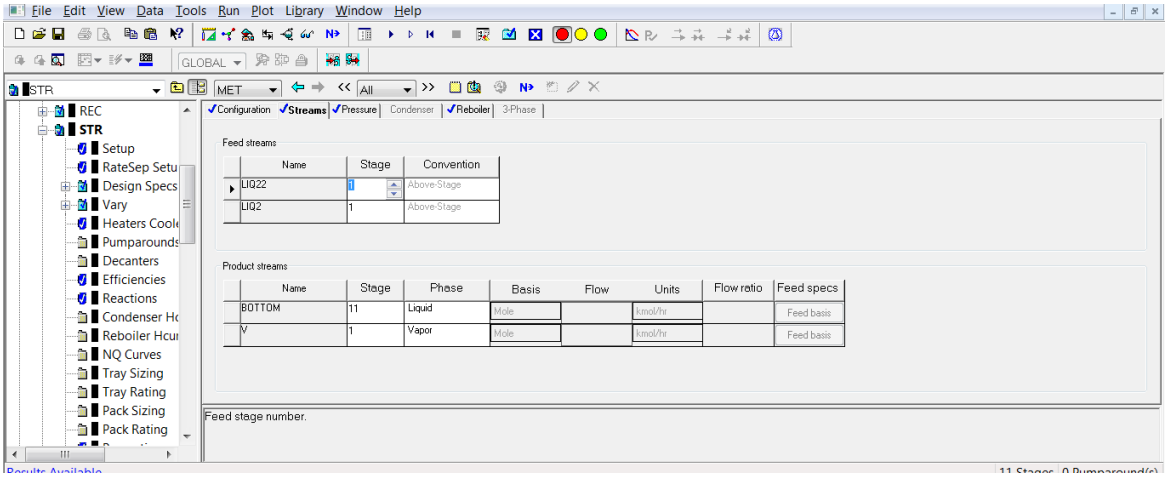


Figure 3.14: specification sheet for block STRIPPER (STREAMS)

The pressure profiles for the stages are entered as shown in Fig 3.15.

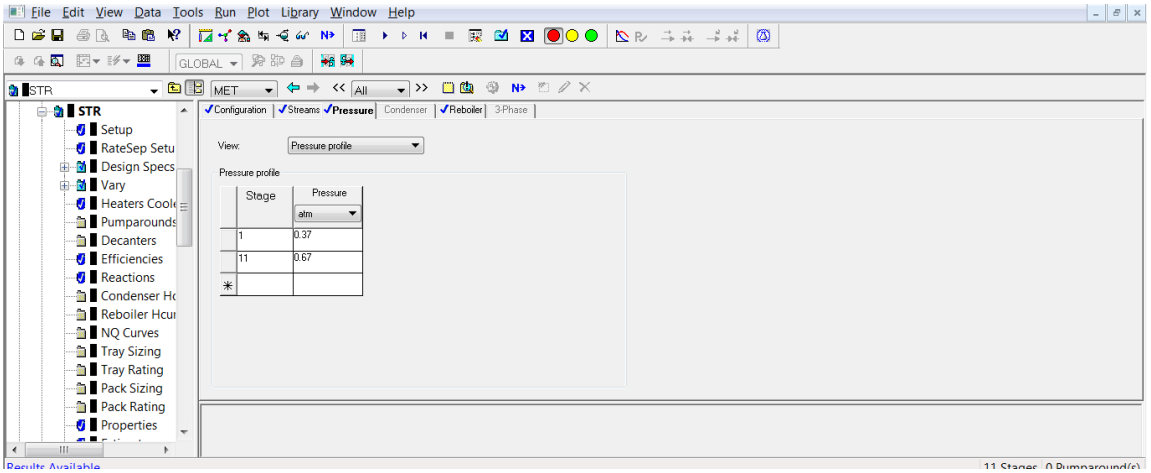


Figure 3.15: specification sheet for block STRIPPER (PRESSURE)

3.3 Equipment Sizing

3.3.1. Length

Height of the column can be calculated, if the numbers of trays are known. The typical distance between trays (tray spacing) is 0.61 m (2 ft). If there are N_T stages, the number of trays is $N_T + 2$ (one stage for the reflux drum and one for the reboiler). In addition to the trays, some space is needed at the top where the reflux piping enters the vessel and at the feed tray for feed distribution piping. More significantly, space is needed at the base to satisfy two requirements: (1) liquid holdup and (2) the liquid height in the base of the column must be high enough above the elevation of the bottoms pump to provide the necessary net positive suction head (NPSH) requirements for this pump. Therefore, a design heuristic is to provide an additional 20% more height than that required for just the trays. So the length of the vessel can be estimated from the following equation.

$$\mathbf{l = 1.2(0.61)}(\boldsymbol{N_T - 2})$$

Here l is the length of the column. Lengths of all blocks were calculated using the above equation. The results for the length of all the blocks are given in Table 3.2.

Table 3.2: Calculated Length of all the four blocks.

BLOCK	No. of stages	Length(in meters)
RECTIFR	12	7.32
STRIPPER	11	6.588
ABSRBR1	24	16.104
ABSRBR2	24	16.104

3.3.2. Diameter

Aspen Plus has an easy-to-use tray sizing capability Tray Sizing which can be used to calculate the diameter of each column. The steps for calculation of diameter for the Block (“RECTIFR”) as shown in Fig. 3.16.

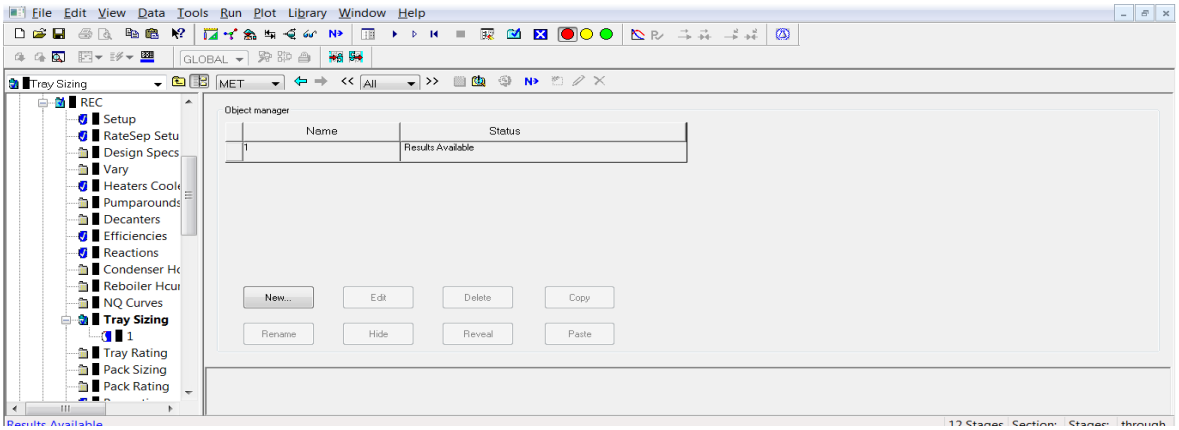


Figure 3.16: specification sheet for RECTIFR (TRAY SIZING)

Under the RECTIFR block tab open the Tray sizing window as shown in Fig. 3.17 and the data was entered after entering the required data the simulation was run.

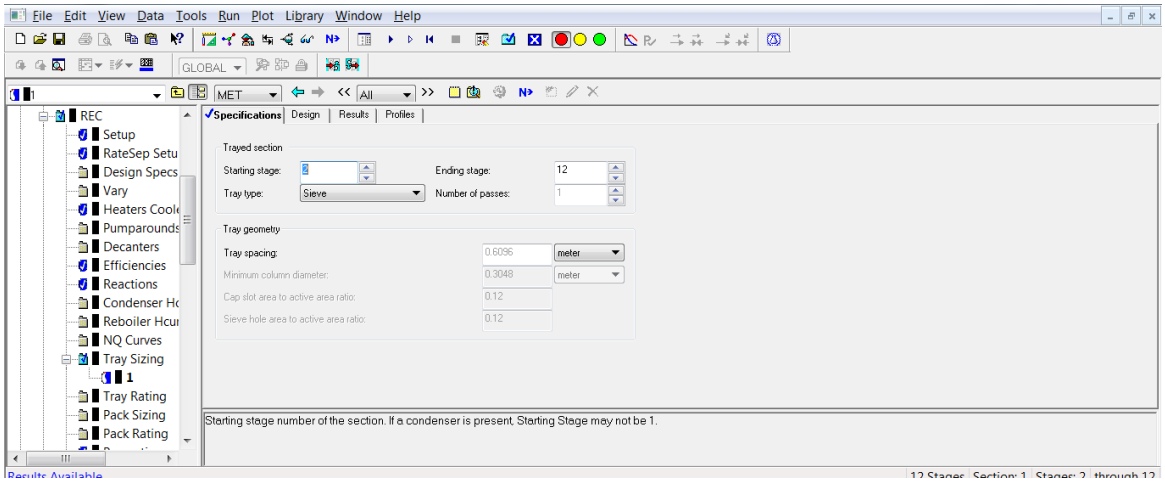


Figure 3.17: Specification sheet for RECTIFR (TRAY SIZING)

Then the results of diameter calculations are viewed in the results tab as shown in Fig 3.18. The results for the diameter of all the blocks are given in Table 3.3.

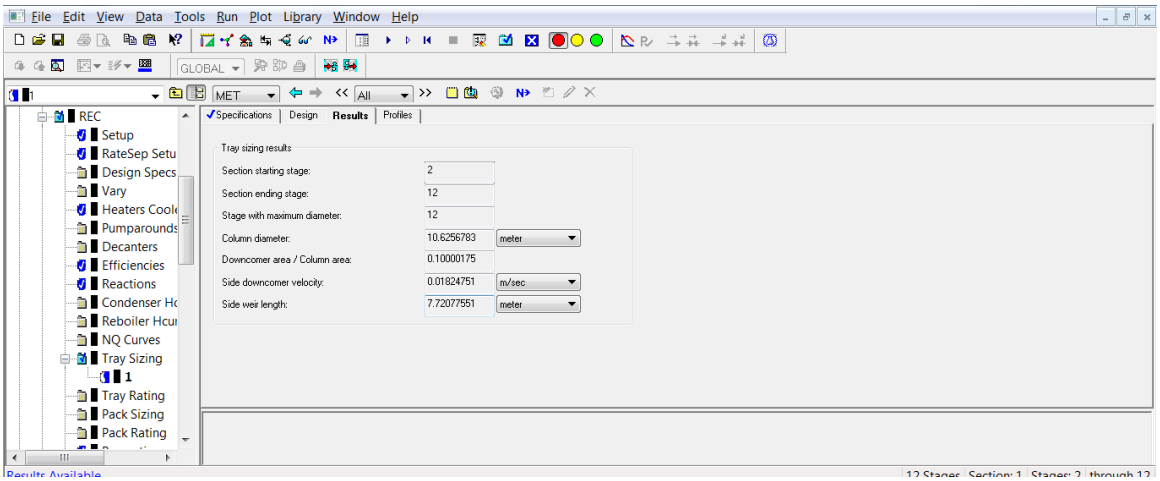


Figure 3.18: Results for diameter of RECTIFR

Table 3.3: Diameter of all Blocks

BLOCK	Diameter (in meters)
RECTIFR	10.625
STRIPPER	10.625
ABSRBR1	8.133
ABSRBR2	7.08

3.3.3. Sizing of reflux drum and sump

The sizes of the reflux drum and the column base were then calculated. A commonly used heuristic is to set these holdups to allow for 5 min of liquid holdup when the vessel is 50% full, based on the total liquid entering or leaving the vessel. For the reflux drum, this is the sum of the liquid distillate and the reflux. For the column base, it is the liquid entering the reboiler from the bottom tray.

The volumetric liquid flow rates can be found by clicking on Profiles under the block RECTIFR and then opening the Hydraulics page tab. Fig.3.19 shows the window that opens on which the volumetric liquid flow rate for the reflux drum (stage 1) was shown. Scrolling down to the bottom tray (stage 12) gave a volumetric liquid flow rate.

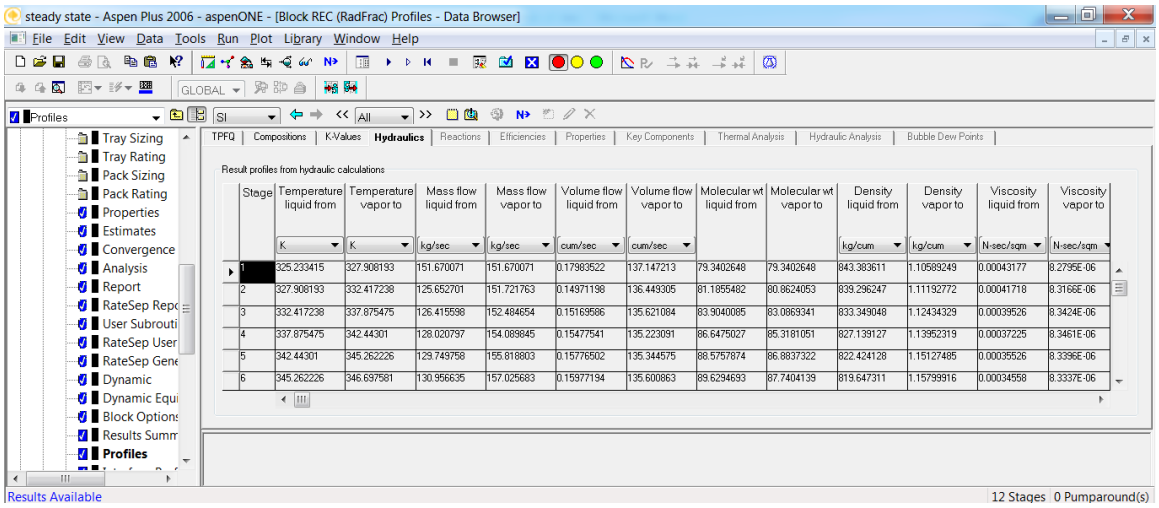


Figure 3.19: hydraulics page tab of RECTIFR showing volumetric flow rate of each stage

Calculations:

The total volume of the reflux drum should be:

$$10.66(60)10 = 6412.86m^3$$

And that of the column base:

$$9.61(60)(10) = 5767.32 \text{ m3}.$$

Assuming a length to diameter ratio of 2, the diameters and lengths can be calculated:

$$\text{Volume} = \frac{\pi}{4}\text{d}^2(2\text{d})$$

The reflux drum is 15.98 m in the diameter and 31.85 m in length. The column base (or reboiler or "sump") has a diameter of 15.43 m and a length of 30.85 m. The Table 3.4 gives the values of diameter and length of all the blocks.

Table 3.4: Dimensions of reflux drum and sump associated with different blocks

BLOCK	REFLUX DRUM		SUMP	
	DIAMETER (m)	LENGTH (m)	DIAMETER (m)	LENGTH (m)
ABSRBR1	-	-	-	-
ABSRBR2	-	-	-	-
RECTIFR	15.98	31.85	15.43	30.8542
STRIPPER	4.252	9.0457	2.7285	5.457

3.4 Dynamic Simulation of DWC

The simulation of DWC dynamic mode was first done in ASPEN PLUS and then it was exported to ASPEN dynamics. The integration of two columns into one shell leads to more interactions among the controlled and manipulated variables, and this affects the controllability of the system. Although much of the literature focuses on the control of binary distillation columns, there are just a few studies on the controllability and dynamic optimization of DWC (Halvorsen et al., 1997; Serra et al., 1999, 2000, 2001; Adrian et al., 2004; Ling et al., 2009, 2010; Diggelen et al., 2010).

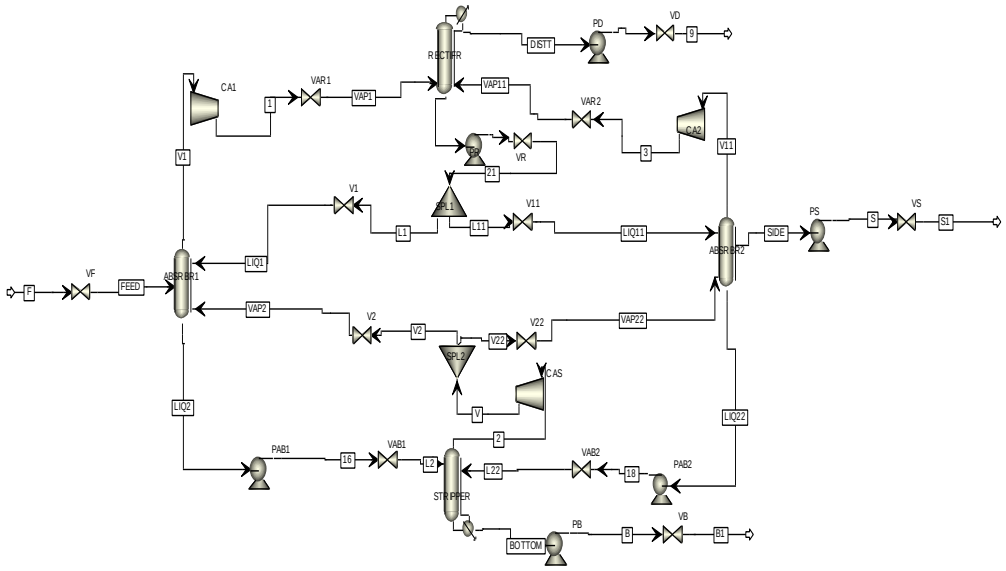


Figure 3.20: Dynamic flow sheet of DWC

The steady state simulation is first converted into the dynamic simulation in ASPEN PLUS. For this we require the results given in Table 3.3 and 3.4 that is the diameter of the column, dimensions of reflux drum and sump. After making the flow sheet as shown in Fig. 3.20 the first specification input sheet which needed to be filled was that of set up. In this sheet we entered input mode as "Dynamic" (Fig. 3.21). Before exporting the file into Aspen Dynamics, a number of important changes had to be made, so the flow sheet was modified as per the requirements in the dynamics by installing the control valves, pumps and the compressors as shown in the Fig. 3.20. in order to obtain a pressure-driven dynamic simulation. The liquid level in the base of the

rectifier corresponds physically to the total liquid trap-out tray. A pump and two parallel lines with control valves in each were installed.

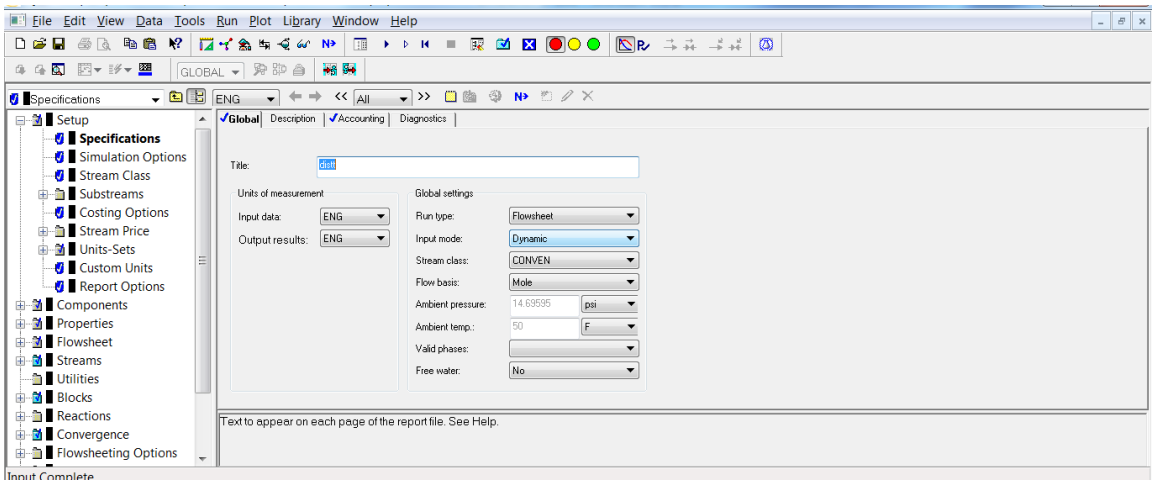


Figure 3.21: Set up specification sheet

The data for feed stream was entered as shown in Fig 3.22.

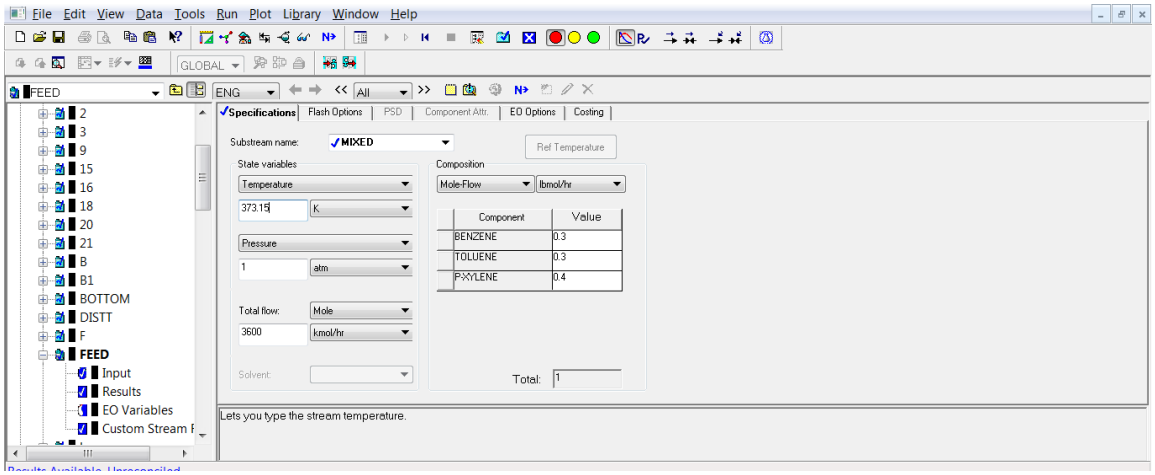


Figure 3.22: Specification sheet for feed stream

The data in the input specification sheets for all the blocks was entered in the same way as was done for the steady state simulation. Except this an additional data of the dynamics sheet needs to be entered, these are the dimensions of the Reflux drum sump and the tray geometry data. These values were entered by clicking the Dynamics button on the top toolbar. On the Reflux Drum page tab, the appropriate diameter and length are entered. The same is done on the Sump page tab (Fig.3.23 and 3.24).

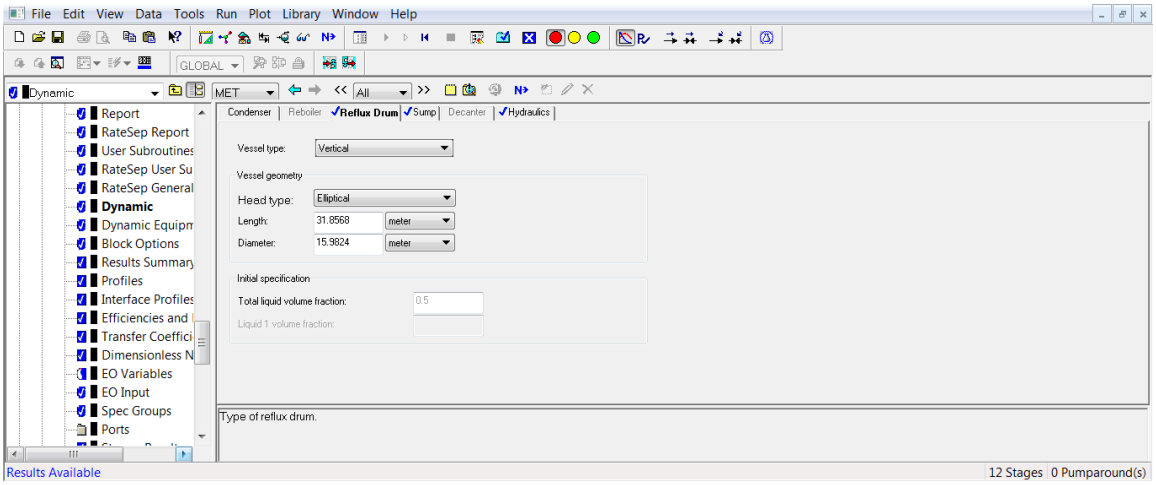


Figure 3.23: Specification sheet for Dimensions of reflux drum

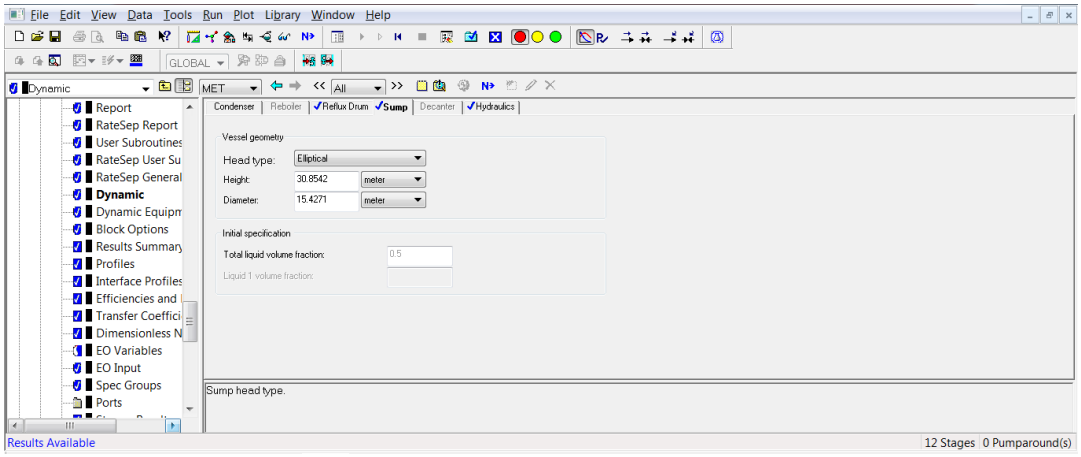


Figure 3.24: Specification sheet for Dimensions of Sump

Finally, the Hydraulics page tab is clicked, and the window shown in Fig.3.25 opens, on which stage numbers and the column diameter were entered. The default values of weir height and tray spacing are 0.05 and 0.6096 m respectively. The data of all blocks “RECTIFR”, “STRIPPER”, “ABSRBR1”, and “ABSRBR2” was entered in the input sheets. After entering all the data for the blocks we needed to enter the data in the valves, pumps and compressors installed in the lines. The input sheet required the data of pressure drop or outlet pressure for these blocks. The data for the outlet pressure was specified by considering the fact that the outlet pressure of the block should be equal to the pressure of the stage on which the stream is entering the other block.

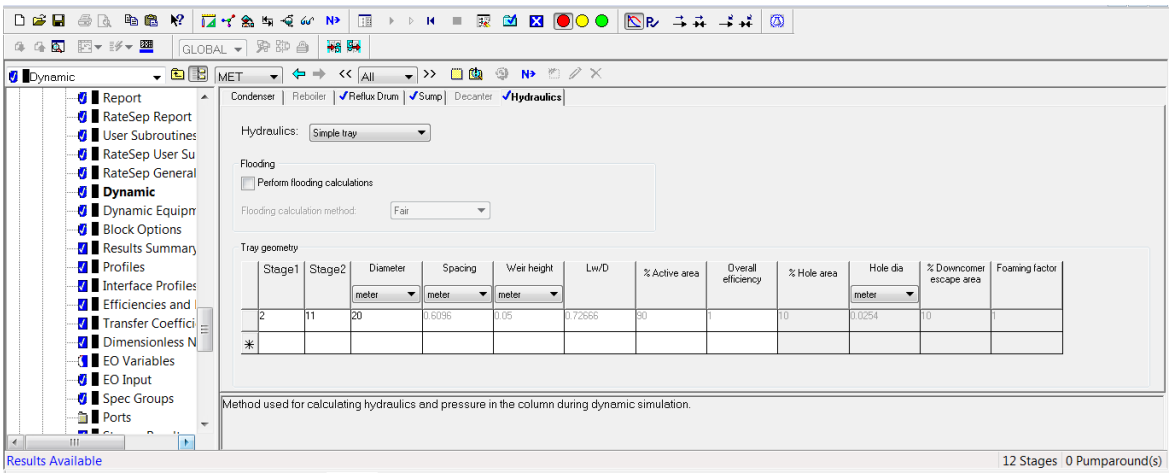


Figure 3.25: Specification sheet of Hydraulics

After entering all the required data the simulation is run. Once the simulation ran without any errors. This simulation was then checked whether it was pressure driven or not by clicking the button  The simulation was then exported to aspen dynamics. By clicking on the button  in the toolbar. The exported file was then opened in the ASPEN DYNAMICS and Fig. 3.26 shows the flow sheet which appeared when the simulation was exported.

3.5 Simulation in ASPEN Dynamics

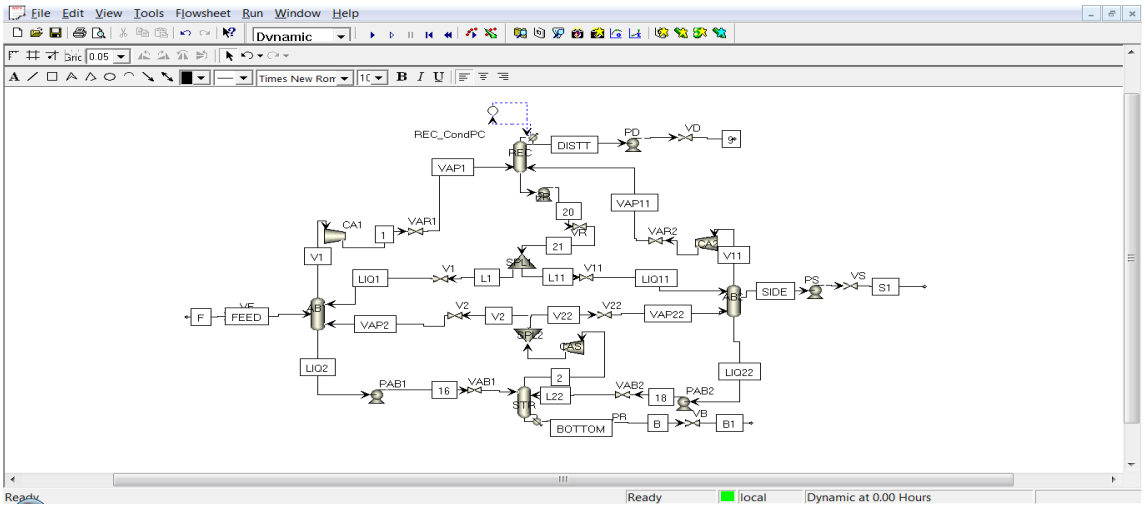


Figure 3.26: Simulation exported to Aspen Dynamics

The set points were chosen for the three product compositions. A control structure was selected. The simplest control structure possible was just an extension of the control of a regular distillation column with a side stream also known as the three-point control structure. In this

control structure the distillate purity (x_{D1}) was controlled by manipulating the reflux rate (L), the side stream Purity (x_{S2}) was con-trolled by manipulating the side stream flow rate (S) and the bottom purity (x_{B3}) was controlled by manipulating the vapor boil up (V). This three-point structure LSV was suggested by Wolff and Skogestad. The controllers used for the control study of the model were PID as PID controllers remain the most used controllers in the chemical industry, for several reasons such as simplicity of the control structure, robustness with respect to model uncertainties.

Based on the results of studies by Diggelen et al., 2010; Kiss and Rewagad, 2011 we considered the best PID configuration (DB/LSV). In this configuration, the liquid levels in the reflux tank and reboiler are maintained by means of D (distillate) and B (bottoms flow rate) whereas the product compositions are maintained by manipulating L(liquid reflux),S (side product flow rate) and V(vapor boil-up) respectively. In case of a DWC subjected to persistent disturbances, the DB/LSV structure was found to be performing the best Kiss and Rewagad, 2011.

After exporting and making first initialization run, the controllers required for the steady state operation of the divide wall distillation column are installed on the blocks. The goal is to maintain the product qualities at their given set points even in the presence of the disturbances.

The manipulated and controlled variables were taken as shown in Table 3.5 (Ling and Luyben; 2009). The controllers installed are shown in Fig. 3.27. Three composition controllers were installed on distillate side stream and the bottom product streams, named as CC1, CC2 and CC3 respectively. We need to include additional dynamic elements in the loop. Composition measurements have significant inherent dynamic lags. A dead time was connected along with these composition controllers to account for the measuring lag. A Flow controller (FLOW C) was installed on the feed stream to control the feed flow rate disturbances. Two level controllers were installed on the condenser for control of liquid level in the reflux drum (LC1) and other on the reboiler to control the liquid level in the sump (LC2).

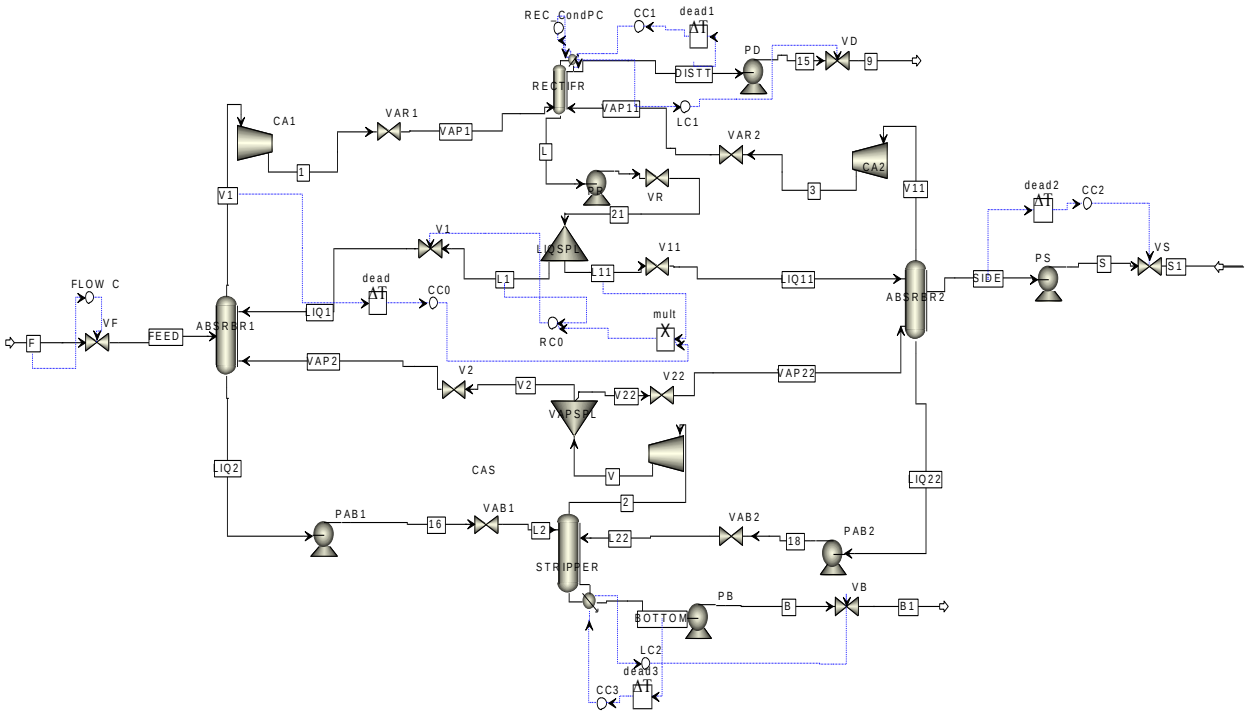


Figure 3.27: Divided Wall Column Control Structure

Any amount of heavy component which goes out the top of the wall would strongly affect the purity of the side stream (S). Similarly, the amount of light component that goes out the bottom of the prefractionator section would also affect the composition of the side stream. Since the side stream is collected as a liquid product, it means that any small amounts of light impurity in the vapor phase will not significantly affect the side stream composition.

Table 3.5: Controlled and manipulated variables for dividing wall column

Controlled variables	**Manipulated variables**
Top product composition	Reflux flow rate
Middle product composition	Side stream flow rate
Bottom product composition	Reboiler heat input
Condenser/accumulator holdup	Distillate stream flowrate
Reboiler holdup	Bottom product flow rate
Heavy component mole fraction in the top of fractionator	Liquid split at top of dividing wall

Even small amounts of heavy key impurity in the liquid phase was also found to upset the side stream composition (Halvorsen and Skogestad 1997, 1999). Based on these considerations, a fourth control loop was added where the liquid split ratio was used to control the level of the heavy impurity in the top of the prefractionator.

The liquid flow rate to the side stream section is measured, and this signal is sent to a multiplier (mult.) whose other input is the output of the composition controller in the prefractionator. The output of the multiplier is the set-point signal to a flow controller (RC0) that manipulates the valve in the liquid line to the prefractionator to achieve the specified flow rate and hence the liquid split is also controlled.

Ling and Luyben, 2009 noted that the ratio of liquid going to the side stream side and the prefractionator side from the rectification section was controlled by the composition controller installed on the prefractionator (CC0). This was an additional loop which was added to manipulate the liquid split in order to control the heavy component composition in the top of fractionators. The installed controllers are shown in the Fig. 3.27.

The data for the set points is entered in the faceplates shown in figure 3.28. The simulation is run in the dynamics mode after installing all the requisite controllers on the blocks of the DWC structure as shown in figure 3.28.

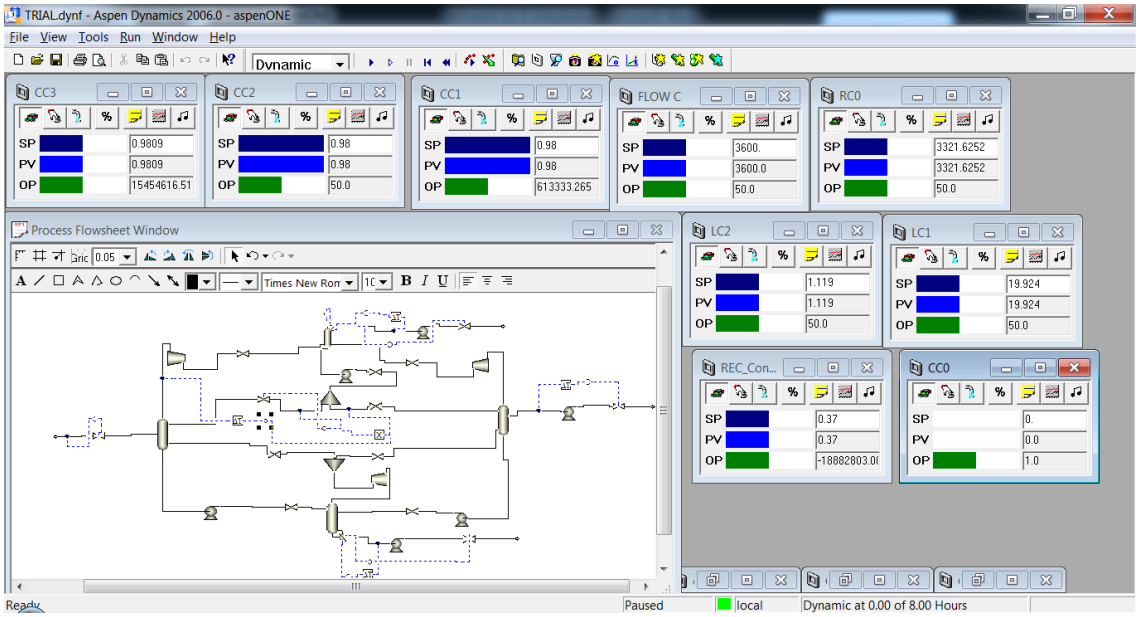


Figure 3.28: Controller Faceplates

The composition control loops each have a 1-min dead time. These controllers were tuned using a sequential method. Since reboiler heat input affects all of the controlled variables fairly quickly, the x_B/Q_Rloop was tuned first with the other controllers on manual. Tyreus-Luyben tuning rules were used to find the ultimate gain and period. Next, since reflux affects all compositions, the x_D/L loop was tuned using the same procedure with the x_B/Q_R loop on automatic. Finally, the x_S/Sloop was tuned with the two loops on automatic (Ling and Luyben, 2009). Table 3.6 give controller tuning results for control loops.

Table 3.6: Controller tuning results for control loops

Controller	Manipulated variable	Controlled variable	Controller Gain (K_C)	Integeral time (τ_I ,minutes)
CC1	x_D	L	238.1214	75.24
CC2	x_S	S	14.2427	132
CC3	x_B	Q_B	1.52	51.48

CHAPTER 4
RESULTS AND DISCUSSION

The simulation results of steady state and dynamics of a DWC are presented in this chapter.

4.1 The Steady State Analysis of DWC

Many investigators reported that the energy requirement of DWC is mainly affected by the operational parameters of DWC (Rangaiah et al., 2009; Sangal et al., 2012c). Sangal et al. (2012b) also noted that operational parameters of DWC are more significant as compared to the structural parameters for the energy requirement of a DWC. So, in the present study we assume that the structural parameters are constant. Separations of BTX mixture are considered as a case study. For steady state simulation, the column, feed and product specification are given in Table 4.1.

Table 4.1: Operating parameters for the BTX separation.

Parameter	Specifications
Feed pressure	1 atm.
Feed flow rate	3600 kmol/hr
Feed composition	Benzene: 0.3 Toluene: 0.3 p-Xylene: 0.4
Product specifications	Benzene: 0.98 Toluene: 0.98 p-Xylene: 0.98
Pressure	Condenser: 0.37 atm. Reboiler: 0.67 atm.
Distillate flow rate	1080 kmol/hr
Side draw flow rate	1080 kmol/hr
Number of stages	47

The steady state simulation converged and then a number of steady state simulations results were carried out to find the optimum liquid and vapor split on the basis of minimum reboiler duty. The simulations were done for obtaining the optimum liquid split for minimizing the reboiler duty, by assuming other parameters constant. After that, the simulations were done for the optimum vapor split for minimizing the reboiler duty. These results were then plotted as liquid split verses the reboiler duty. Fig. 4.1 shows the variation of reboiler duty w. r. to liquid split. It is clear from

Fig. 4.1 that the reboiler duty first decreases, reaches an optimum point and then starts increasing again. The optimum liquid split for minimum reboiler duty is 0.45. Fig. 4.2 shows the variation of reboiler duty w. r. to vapor split. The reboiler duty first decreases, reaches an optimum point and then starts increasing again. The optimum vapor split for minimum reboiler duty is 0.603.

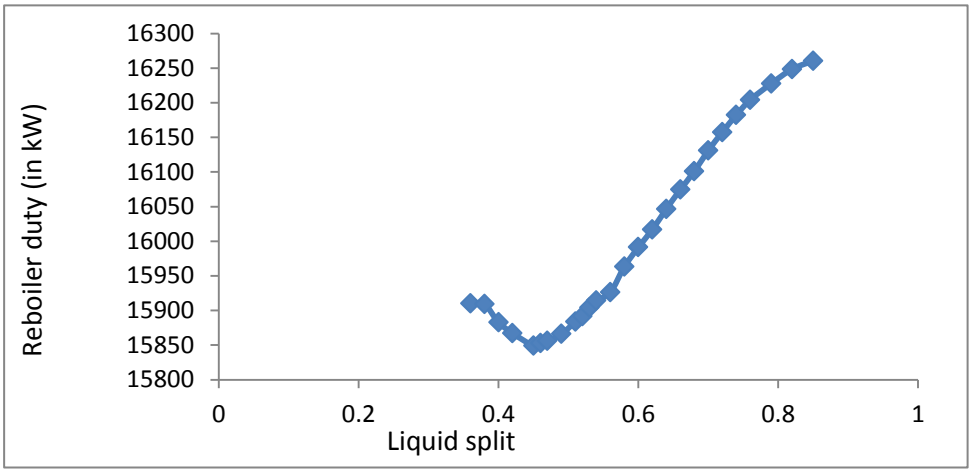


Figure 4.1: variation of reboiler duty with liquid split

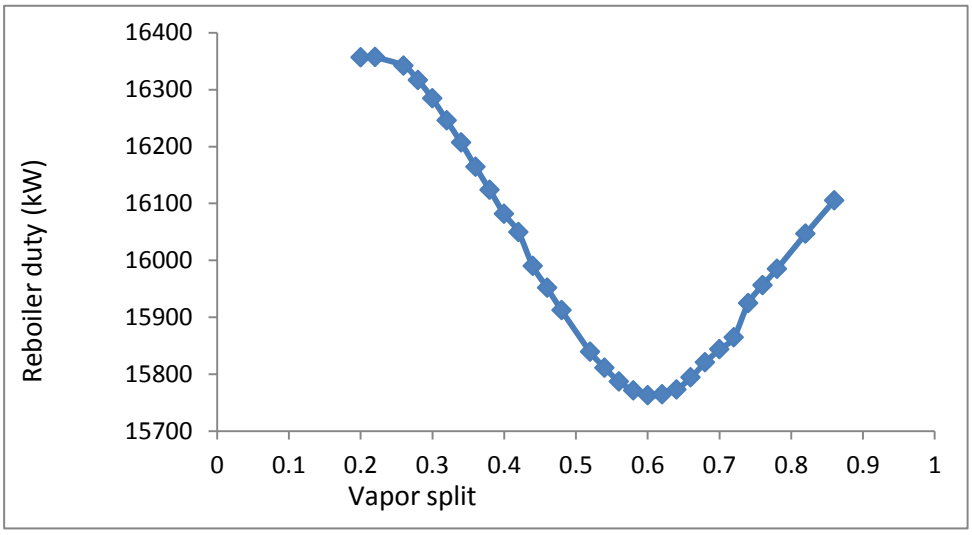


Figure 4.2: variation of reboiler duty with vapor split

Fig. 4.3 shows the variation of reboiler duty with the reflux ratio. The reboiler duty increases as the reboiler duty increases.

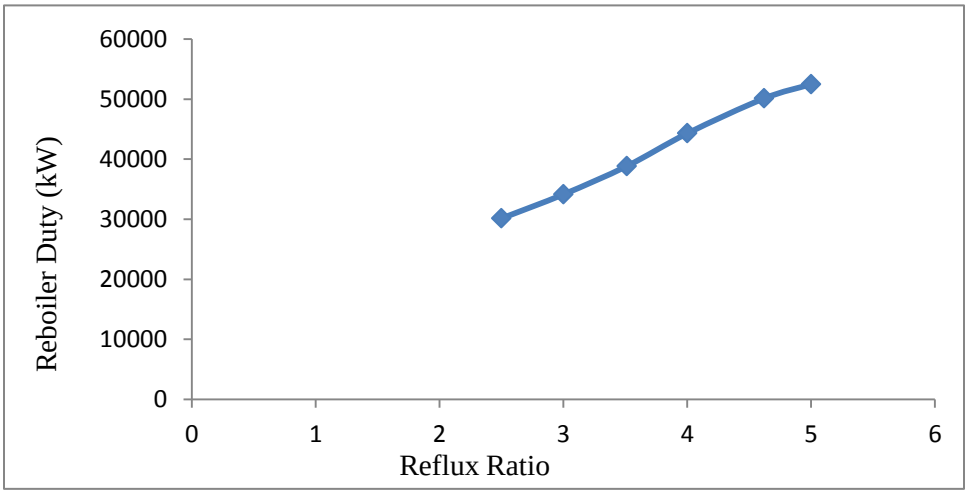


Figure 4.3: Variation of reboiler duty with reflux ratio

At the optimum liquid and vapor split ratio the reflux ratio are 4.63 for achieving the 98% product purity. At the optimum conditions the reboiler duty is 15770 kW.

4.2 Temperature and Composition Profiles within Columns at Optimum Liquid and Vapor Split

The stage wise variation of temperature and the liquid composition for the different blocks of the current study were observed as shown in Fig. 4.4 - 4.5. These results were for the optimum liquid split of 0.603 and the vapor split as 0.45. This value of liquid split was optimized by minimizing reboiler duty which was found to be 15770 kW.

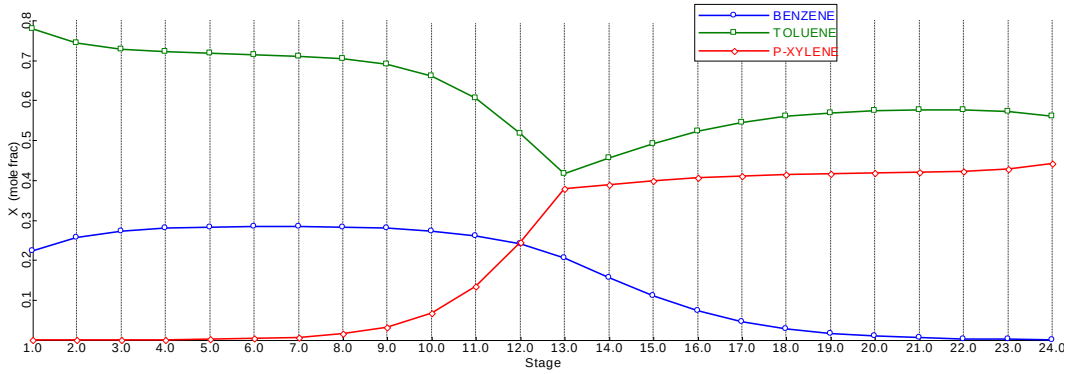


Figure 4.4: Liquid composition profile in block ABSRBR1

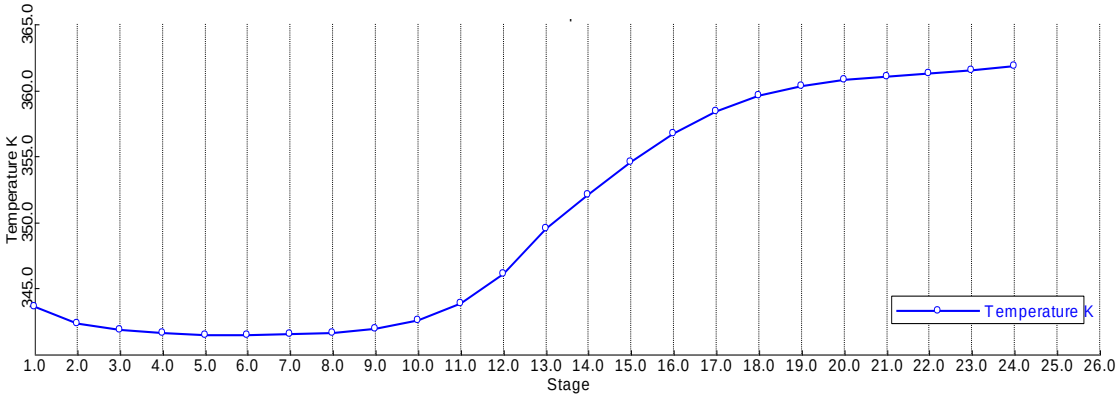


Figure 4.5: Temperature profile in block ABSRBR1

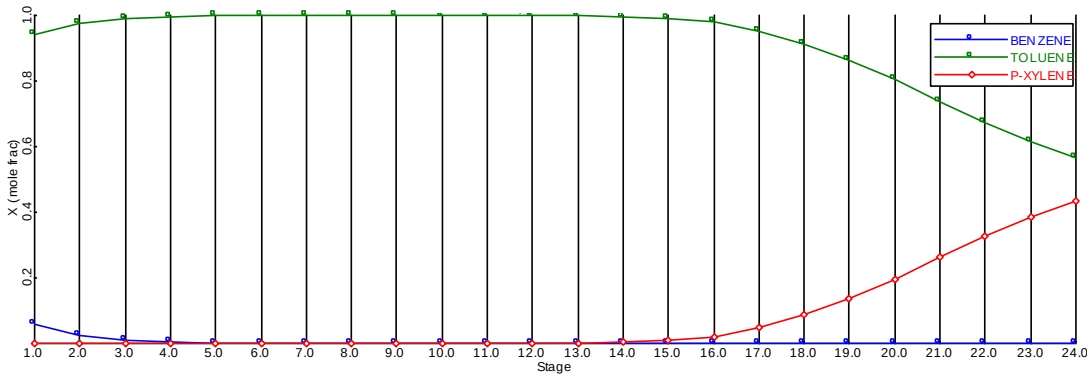


Figure 4.6: Liquid composition profile in block ABSRBR2

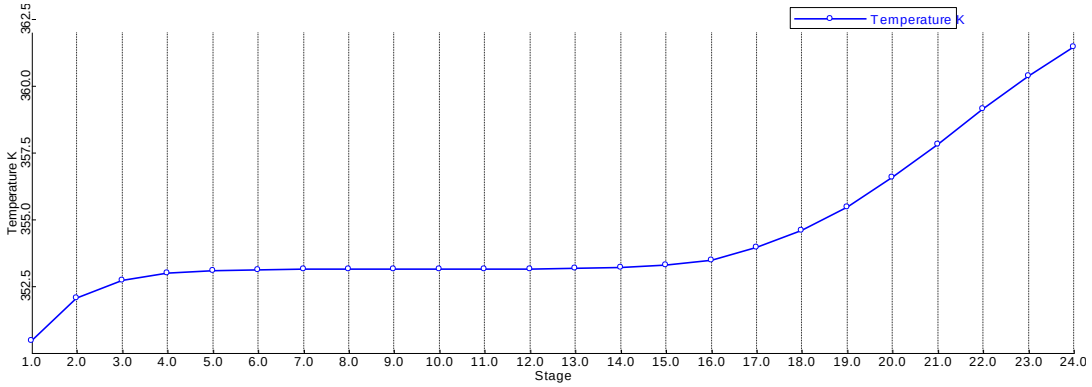


Figure 4.7: Temperature profile in block ABSRBR2.

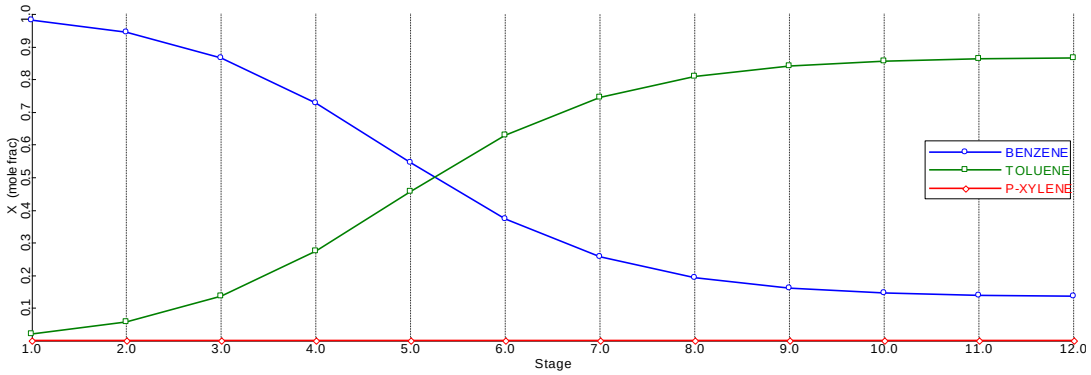


Figure 4.8: Liquid composition profile in block RECTIFR

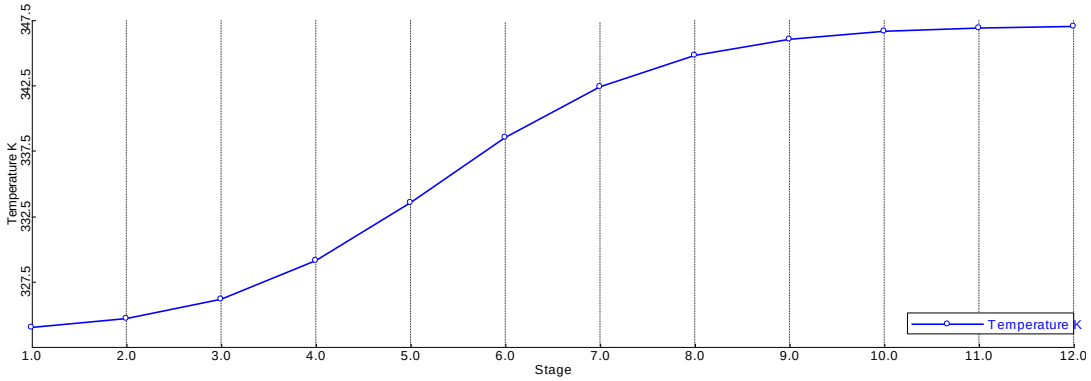


Figure 4.9: Temperature profile in block RECTIFR

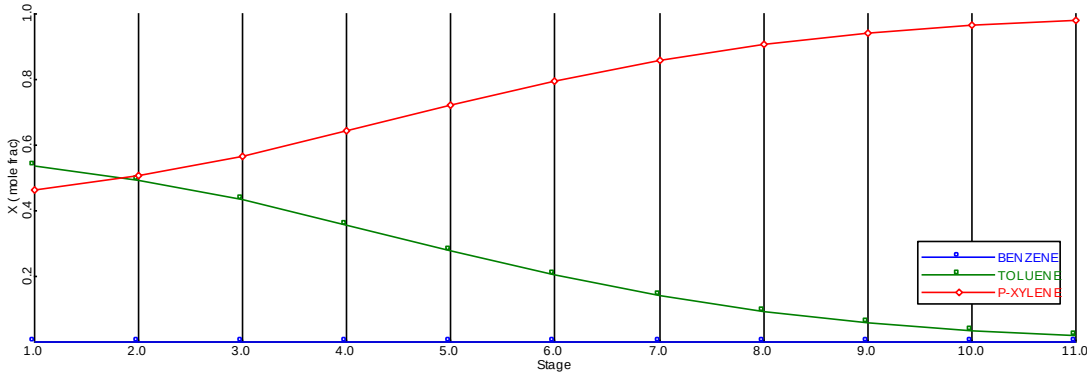


Figure 4.10: Liquid composition profile in block STRIPPER

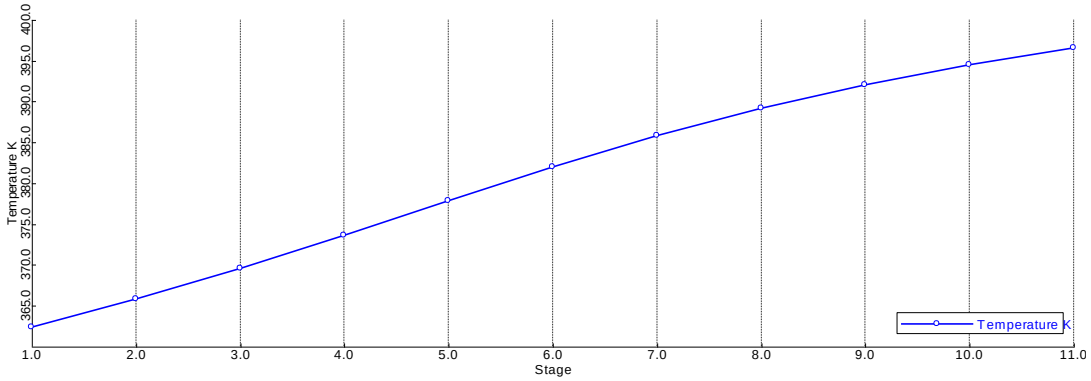


Figure 4.11: Temperature profile in block STRIPPER

4.3 Dynamic Results

Simulations were carried out to study the control behavior of a DWC. The simulation was first done in the ASPEN PLUS in dynamic mode, the required parameters were calculated and are shown in Table 3.2-3.4. The controlled and manipulated variables for dividing wall column parameters used in the study are given in Table 3.5. The simulation was done in ASPEN dynamics. The inputs required for the simulation are the controller tuning parameters of the controllers are given in Table 3.6. The purity set points (SP) were taken as 98% each for distillate, side and bottom product. The disturbances of ±10% in the feed flow rate (F) were used (Fig. 4.12 and 4.13). Even when the disturbances are exerted at the same time, no serious problems such as lack of capability to reach the set points were observed, as illustrated by the figures as follows. The Fig. 4.14 to 4.19 show the results when the feed composition is changed by increasing or decreasing the concentration of one of the components, with the other two components remaining in the initial ratio to each other. The purities of all three products are well controlled.

4.3.1. Results for the feed flow rate disturbances

The results for the disturbances in the ±10% feed flow rate are shown in Figure 4.12. The disturbance is introduced in the feed flow rate after steady state is achieved at time 3 hours (Fig. 4.12a, Fig. 4.13a). The results show that the benzene composition in the distillate and the p-Xylene in the bottom product are not affected to a large extent (Fig. 4.12b, Fig.4.12d, Fig 4.13b, Fig 4.13d). The disturbance affects the composition of Toluene in the side stream (Fig. 4.12c, Fig. 4.13c) but it returned to the set point within one hour.

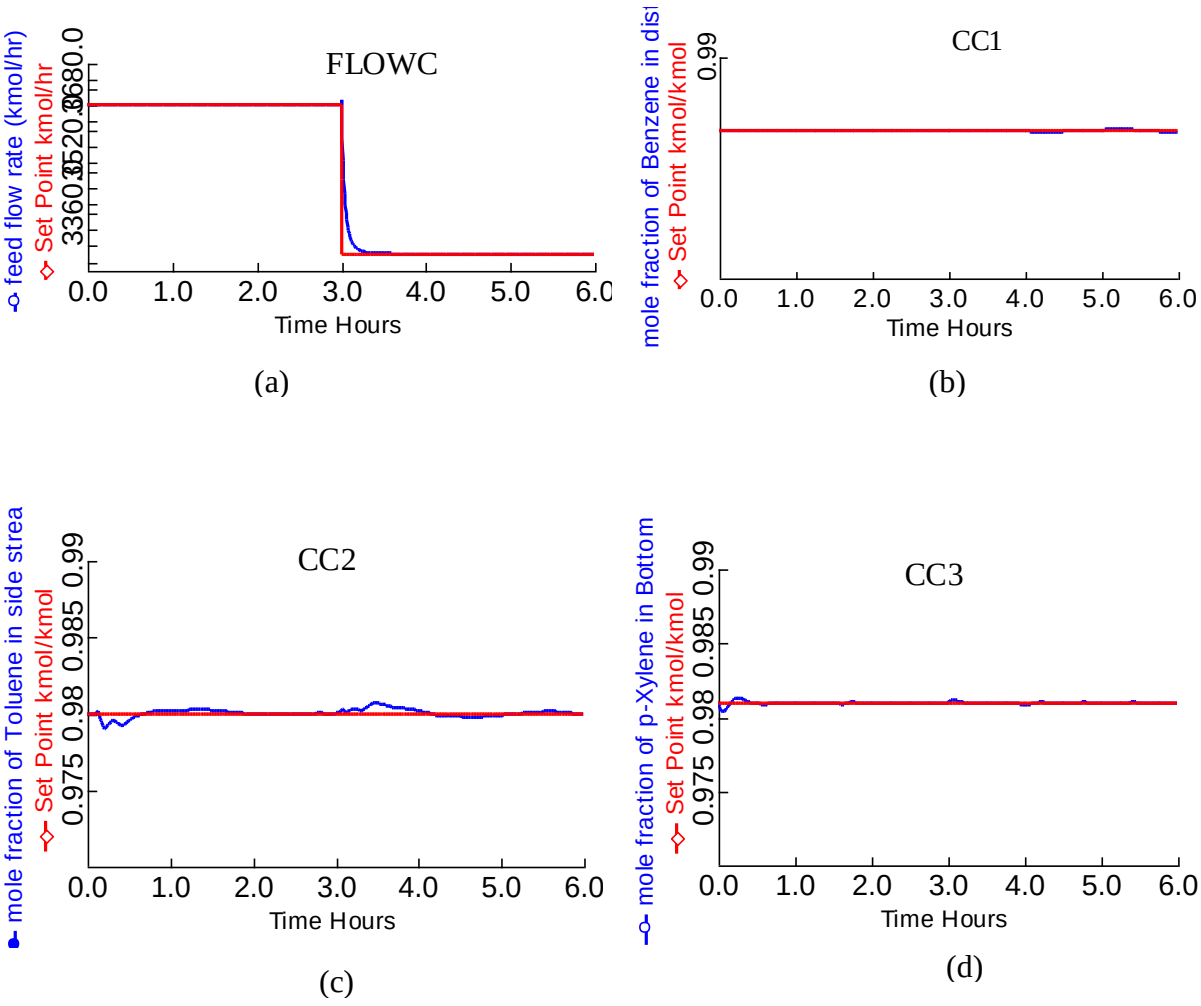


Figure 4.12*:* (a) Feed flow rate plot showing -10% disturbances in F, introduced after 3 hours, (b) plot of the response of composition controller installed in the distillate stream, (c) response of the composition controller installed in the bottom stream, (d) response of the composition controller installed in the side stream.

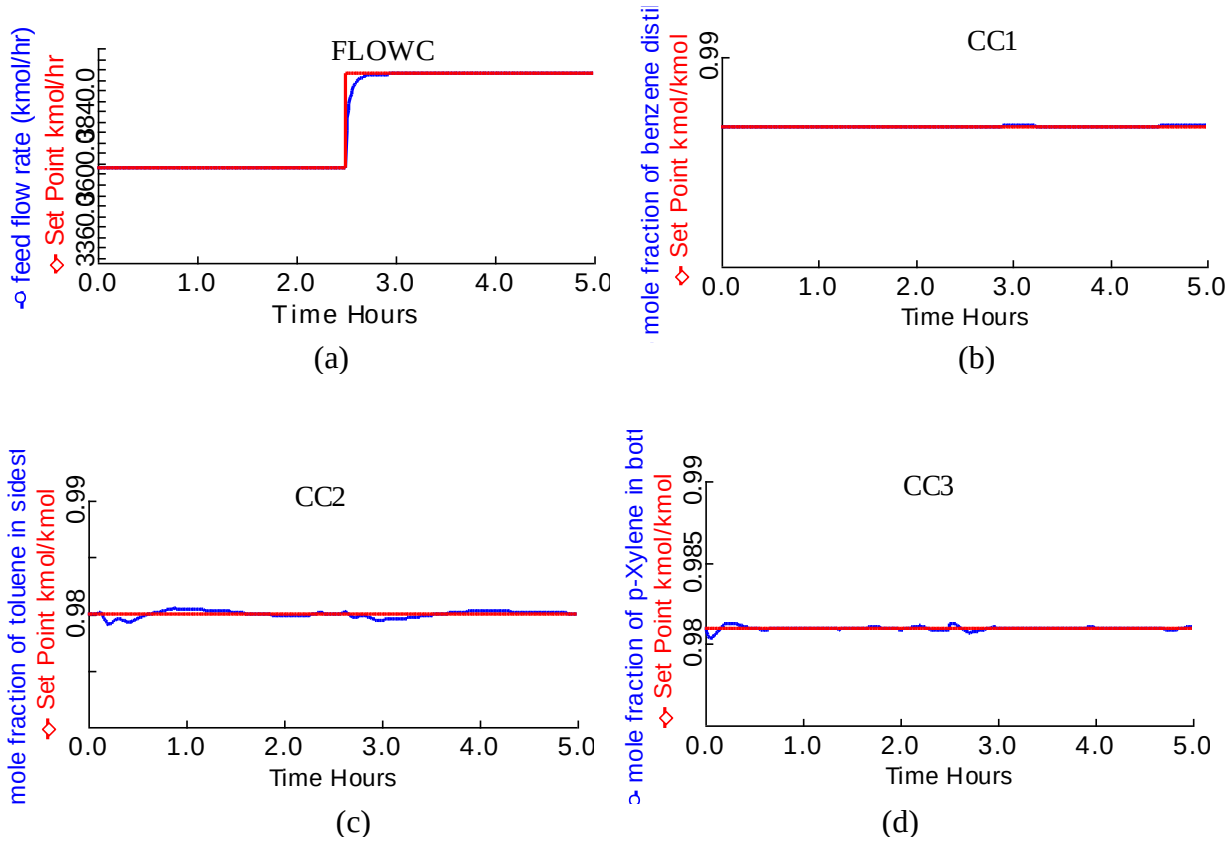


Figure 4.13: (a) Feed flow rate plot showing +10% disturbance in F introduced after 3 hours, (b) plot of the response of composition controller installed in the distillate stream, (c) response of the composition controller installed in the bottom stream, (d) response of the composition controller installed in the side stream.

4.3.2. Results for disturbances in the feed composition

The next step to study the control behavior was to introduce a disturbance in feed composition. The results for the disturbances in the ±5% disturbance in benzene are shown in Fig 4.14 and Fig.4.15. The disturbance is introduced in the mole fraction of benzene after steady state is achieved at time 3 hours. The results show that the feed flow rate remains unaffected by the feed composition disturbance (Fig. 4.14b, Fig. 4.15b). The results obtained also show that the benzene composition in the distillate and the p-Xylene in the bottom product are not affected to a large extent (Fig. 4.14c, Fig.4.14e, Fig 4.15c, Fig. 4.15e). The disturbance affects the composition of

Toluene in the side stream (Fig. 4.14d, Fig. 4.15d) but it returned to the set point within one hour.

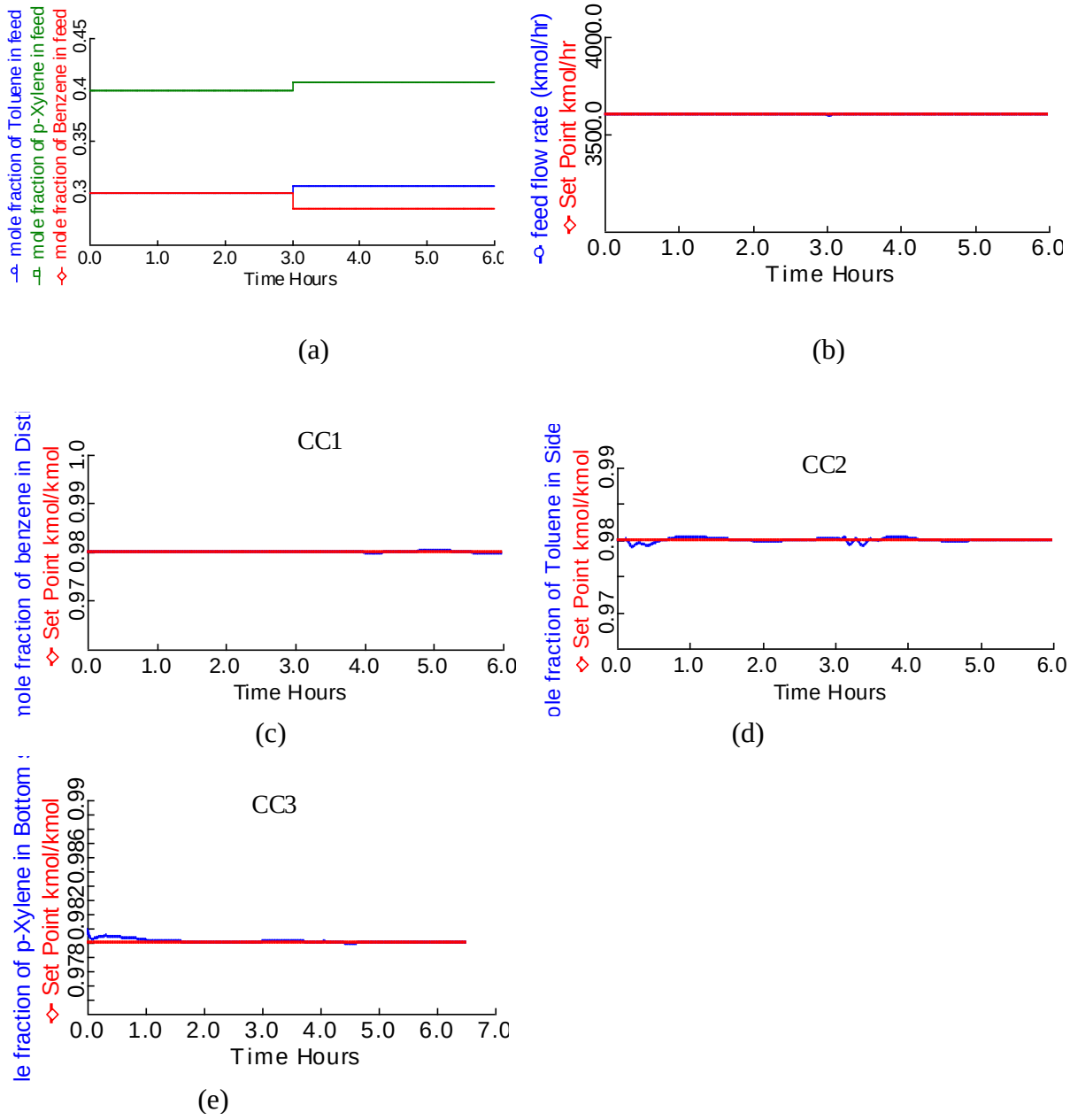


Figure 4.14: (a) Plot showing -5% disturbance in benzene introduced after 3 hours, (b) response of flow controller, (c) plot of the response of composition controller installed in the distillate stream, (d) response of the composition controller installed in the bottom stream, (e) response of the composition controller installed in the side stream.

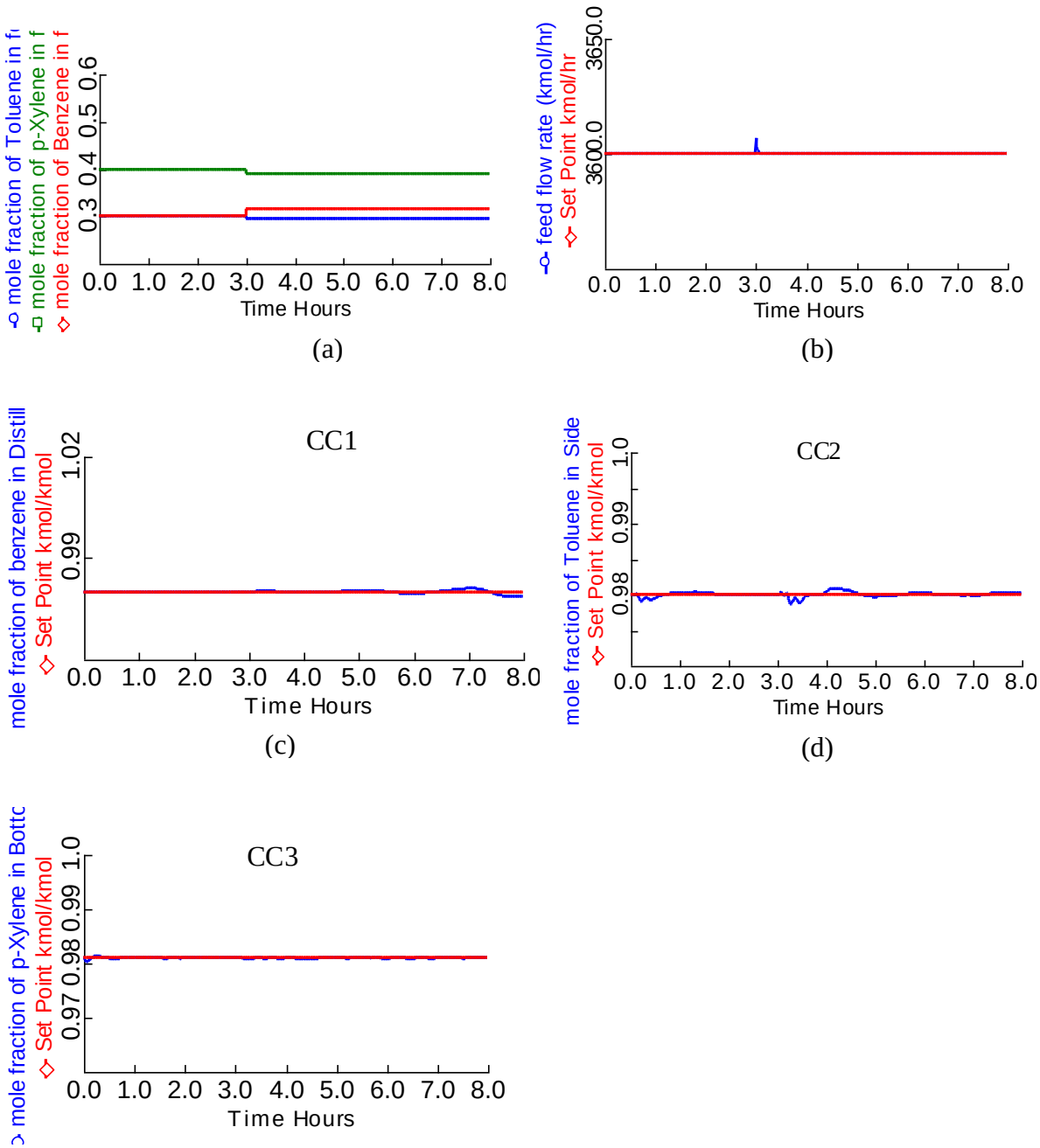


Figure 4.15*:* (a) plot showing +5% disturbance in benzene introduced after 3 hours, (b) response of flow controller, (c) plot of the response of composition controller installed in the distillate stream, (d) response of the composition controller installed in the bottom stream, (e) response of the composition controller installed in the side stream.

The results for the disturbances in the +5% disturbance in p-Xylene are shown in Fig 4.16 and -5% disturbance in p-Xylene are shown in Fig.4.17. The disturbance is introduced in the mole

fraction of p-Xylene after steady state is achieved at time 3 hours. The results show that the feed flow rate (Fig. 4.16b, Fig.4.17b) and the benzene composition in the distillate (Fig. 4.16c, Fig.4.17c) remain unaffected by the feed composition disturbance. However the p-Xylene in the bottom product took a 4 hours to return to the set point (Fig 4.16c, Fig. 4.17c). The disturbance affects the composition of Toluene in the side stream (Fig. 4.16d, Fig. 4.17d) it took 2 hours for the composition to return to the set point.

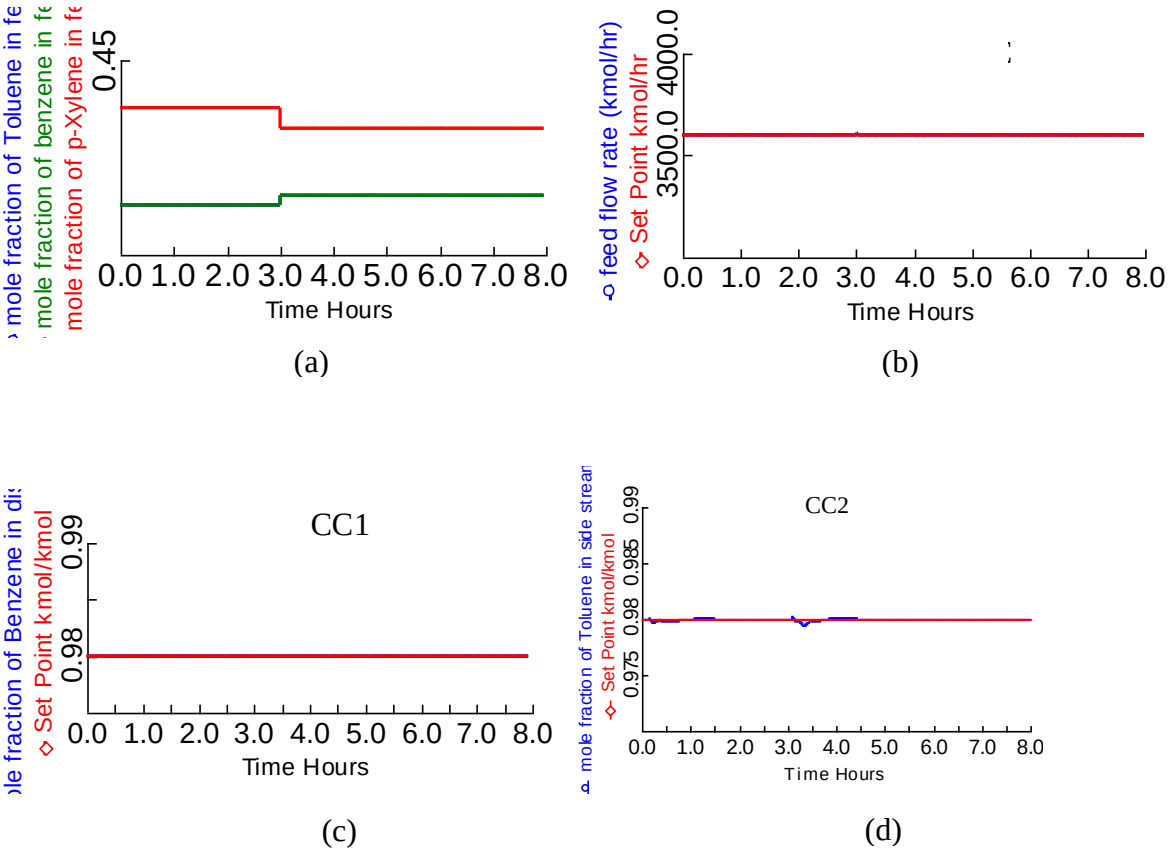
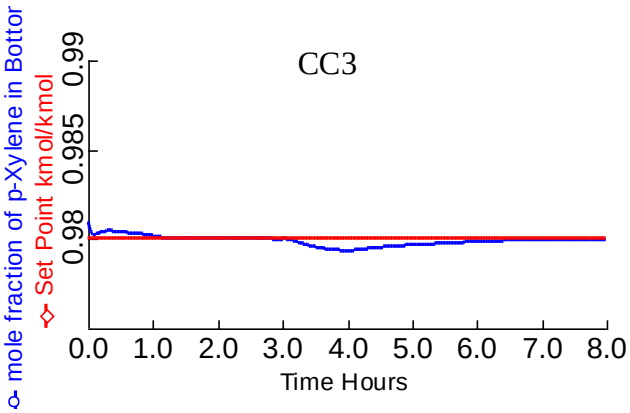
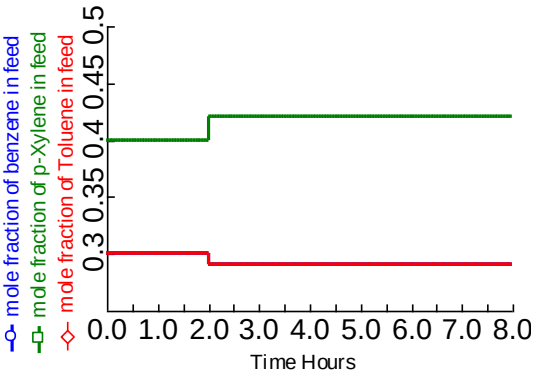


Figure 4.16: (a) Plot showing -5% disturbance in p-Xylene composition in feed introduced after 3 hours, (b) the response of feed flow controller, (c) response of the composition controller installed in the distillate stream, (d) response of the composition controller installed in the side stream.

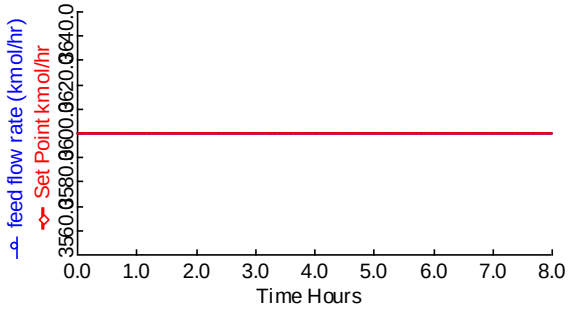


(e)

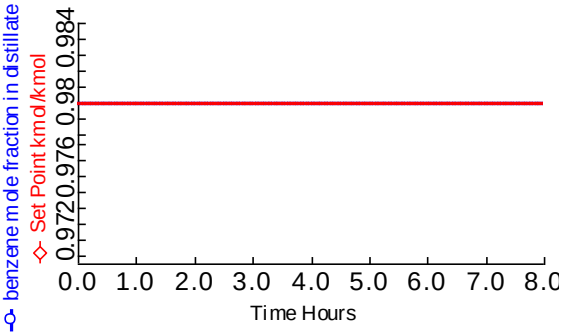
Figure 4.16: (e) response of the composition controller installed in the bottom stream



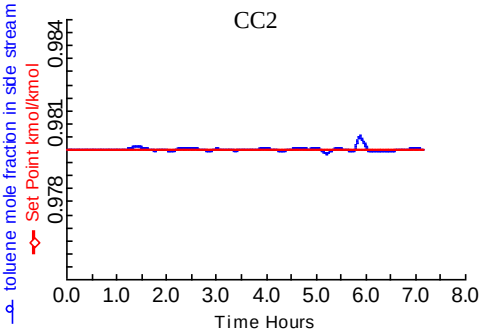
(a)



(b)

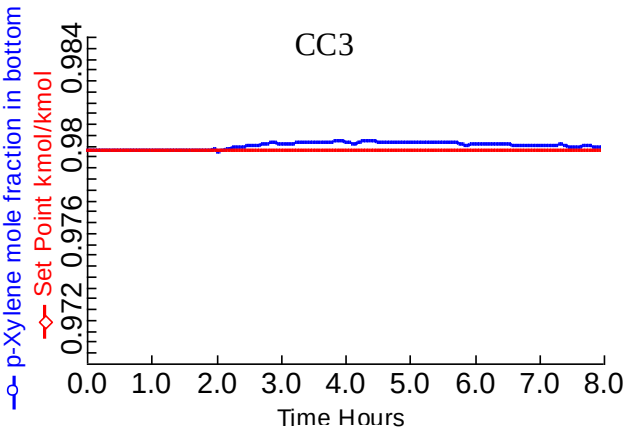


(c)



(d)

Figure 4.17*:* (a) Plot showing +5% disturbances in p-Xylene composition in feed introduced after 2 hours, (b) the response of feed flow controller, (c) response of the composition controller installed in the distillate stream, (d) response of the composition controller installed in the side stream,



(e)

Figure 4.17: (e) response of the composition controller installed in the bottom stream

The results for the disturbances in the +5% disturbance in Toluene are shown in Fig. 4.18 and -5% disturbance in Toluene are shown in Fig. 4.19. After steady state is achieved the disturbance is introduced in the mole fraction of Toluene at time 3 hours. The results show that the feed flow rate (Fig. 4.18b, 4.19b), the benzene composition in the distillate (Fig. 4.18c, Fig.4.19c) and the p-Xylene in the bottom product (Fig. 4.18e, Fig.4.19e) remains unaffected by the feed composition disturbance. However the Toluene in side product took 2 hours to return to the set point (Fig. 4.19d).

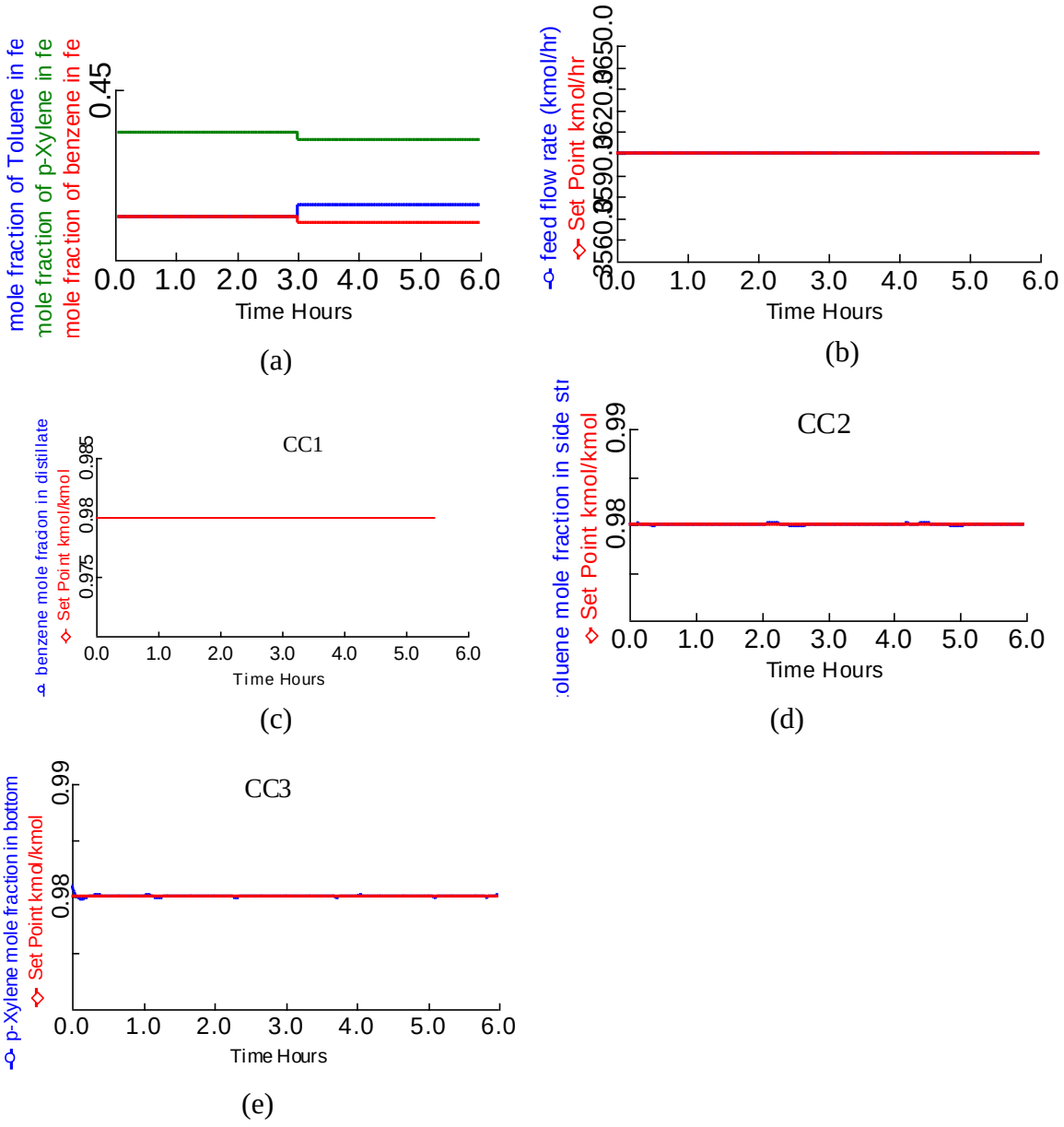


Figure 4.18*:* (a) Plot showing +5% disturbances in Toluene composition in feed introduced after 3 hours, (b) the response of feed flow controller, (c) response of the composition controller installed in the distillate stream, (d) response of the composition controller installed in the side stream, (e) response of the composition controller installed in the bottom stream.

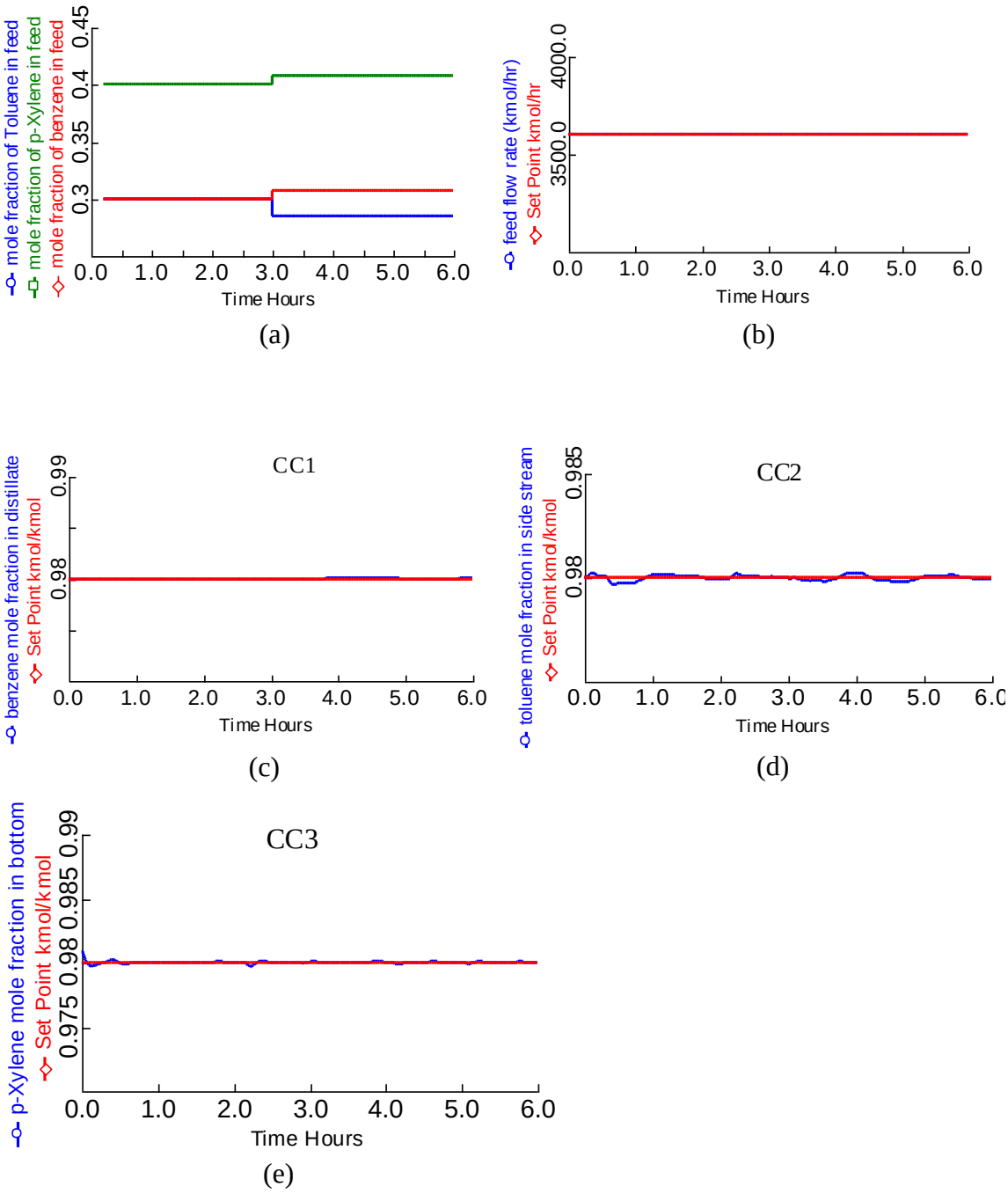


Figure 4.19*:* (a) Plot showing -5% disturbances in Toluene composition in feed introduced after 3 hours, (b) the response of feed flow controller, (c) response of the composition controller installed in the distillate stream, (d) response of the composition controller installed in the side stream, (e) response of the composition controller installed in the bottom stream.

CHAPTER 5
CONCLUSION AND RECOMMENDATIONS

From this study the following conclusion are drawn:

1. For minimizing the energy requirement (reboiler duty) the optimum liquid and vapor split ratio are 0.45 and 0.603 respectively, for the BTX ternary system.

2. At the optimum liquid and vapor split ratio the reflux ratio are 4.63 for achieving the 98% product purity.

3. For minimizing the energy requirements the control structure enhanced by adding an extra loop that controlled the heavy component composition in the top of the prefractionator, by using the liquid split as an additional manipulated variable.

4. The reboiler heat input affected all of the controlled variables quickly; so the composition controllers tuned using a sequential method, using Tyreus-Luyben tuning rules to find the ultimate gain and period.

5. The composition of benzene in the distillate and p-Xylene in the bottom stream remain unaffected when disturbances are introduced in the feed flow rate.

6. The toluene concentration in the product streams returned to the set point after one hour when ±10 % disturbance in feed flow rate.

7. The toluene concentration in the product streams returned to the set point after two hours for ±5% disturbance in benzene, toluene and p-Xylene composition in the feed.

Recommendations and future scope:

1. The study of quaternary and higher order systems in DWC with more than one wall represent an interest for future research.

2. Mixture with different relative volatilities will be analyzed for simulation study of a DWC.

3. The important issue is process integration within a large plant. The results of thermally coupled columns/DWC should be integrated in the process integration toolboxes.

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