Modeling and Simulation Of Ortho Meta Xylene Splitter using Aspen Hysys

A project report submitted in partial fulfillment of the requirements for the

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MASTER OF TECHNOLOGY

In

Refining and Petrochemical Engineering

(Academic Session 2004-06)

By
Pramod Kumar Sahoo
(R080204006)

Under the supervision
Of
Dr. D.N.Saraf
(Distinguished Professor)

COLLEGE OF ENGINEERING STUDIES

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

DEHRADUN (U.A) 248007

MAY 2006

Dedicated

To

My Mother

CERTIFICATE

This is to certify that the project report on **"Modeling and Simulation Of Ortho Meta Xylene Splitter using Aspen Hysys"** submitted to University of Petroleum and Energy Studies, Dehradun by Mr. Pramod Kumar Sahoo, in partial fulfillment of the requirement for the award of degree of Master of Technology in *Refining and Petrochemical engineering* (Academic session 2004-06) is a bonafide work carried out by him under my supervision and guidance. This work has not been submitted anywhere else for any degree or diploma.

Date: May 15, 2006.

Dr.D.N.Saraf

(Distinguished Professor)

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Pramod Kumar Sahoo
Pramod Kumar Sahoo
M.Tech (Refining & Petrochemical Engineering)
Roll no.R080204006
Dehradun

CONTENTS

NOTATION

VARIABLES

D   Distillate rate

E   Equilibrium relation

f   Feed of each component / fugacity

F   Feed rate

G   Vapor rate/ amount of gas

h   Molar enthalpy of liquid

H   Molar enthalpy of vapor

K   Distribution coefficient

l   Molar flow rate of component in liquid phase

L   Total Molar flow rate in liquid phase

M   Discrepancy factor

N   Number of trays

P   Pressure

Q   Heat duty

R   Reflux ratio

T   Temperature

v   Molar flow rate of component in vapor phase

V   Total Molar flow rate in vapor phase

W   Bottom or residue rate

x   Mole fraction in liquid phase

y   Mole fraction in vapor phase

Z   Mole fraction

SUBSCRIPTS

C   Components

D   Distillate

f   Feed tray

F   Feed

G   Gas

hk   Heavy key component

i   Interface / any component

j   Number of stages

lk   Light key component

m   Minimum

t   total

SUPERSCRIPTS

F   Feed

L   Liquid

V   Vapor

GREEKLETTERS

α Relative volatility

Φ Root of equation / fugacity coefficient

μ Viscosity

EXECUTIVE SUMMARY

A steady state mathematical model has been developed for an Ortho Meta Xylene Splitter(OMS). This is basically a simple, multi-component, multi-stage, continuous distillation column and we have simulated it using Naphthali Sandholm method. The equations involved in this mathematical model are non-linear algebraic equations and can be solved by Newton-Raphson method. In the present study simulation has done by Aspen HYSYS 2004 Version, which provides flexibility in products quality, duties, temperature, pressure, liquid to vapor ratio etc. We also used a short-cut method to check the results by hand calculation. The developed models have validated using plant data from an operating unit in BRPL, Bongaigaon. Subsequently we carried out Sensitivity study of the column varying different operating condition such as reflux ratio, pressure temperature, feed, distillate and bottom product flow rate, etc.

INTRODUCTION

In a refinery, a reformer is used to catalytically convert nonromantic to aromatics. The out put from the reformer unit is sent to a stabilizer where lighter hydrocarbon up to C_4 are removed from the top and the bottom of the stabilizer sent to deheptanizer. Where light reformate up to C_7 is removed and the bottom product of the deheptanizer known as C_8^+ reformate, is sent to OMS as feed. The feed for Ortho – meta splitter (OMS) is coming from both C_8^+ isomerisate and C_8^+ reformate. Similarly, the bottom product of deheptanizer in isomerisation unit is known as C_8^+ isomerisate, also feed stock for OMS. OMS feed mainly contain Ethyl Benzene, Ortho-Xylene, Meta-Xylene, Para Xylene and some amount of saturate (C_8, C_9), toluene and C_9^+ aromatics.

The main objective of OMS (fig.1) is to prepare suitable feed for parex unit. Suitable feed means to make Zero percentage C_9^+ aromatics. It is essential because this feed is passed through molecular sieves in parex unit. If minute quantity of C_9^+ aromatics present, it will block on the surface of the sieves. As a result the process will slow down and finally may stop. The overhead product of OMS is sent to parex unit as feedstock and bottom product of OMS sent to Ortho rerun column, where Ortho and C_9^+ aromatics separated. To check C_9^+ aromatics in OMS distillate, on-line analyzer is present in reflux stream of OMS distillate.

ORTHO META SPLITTER
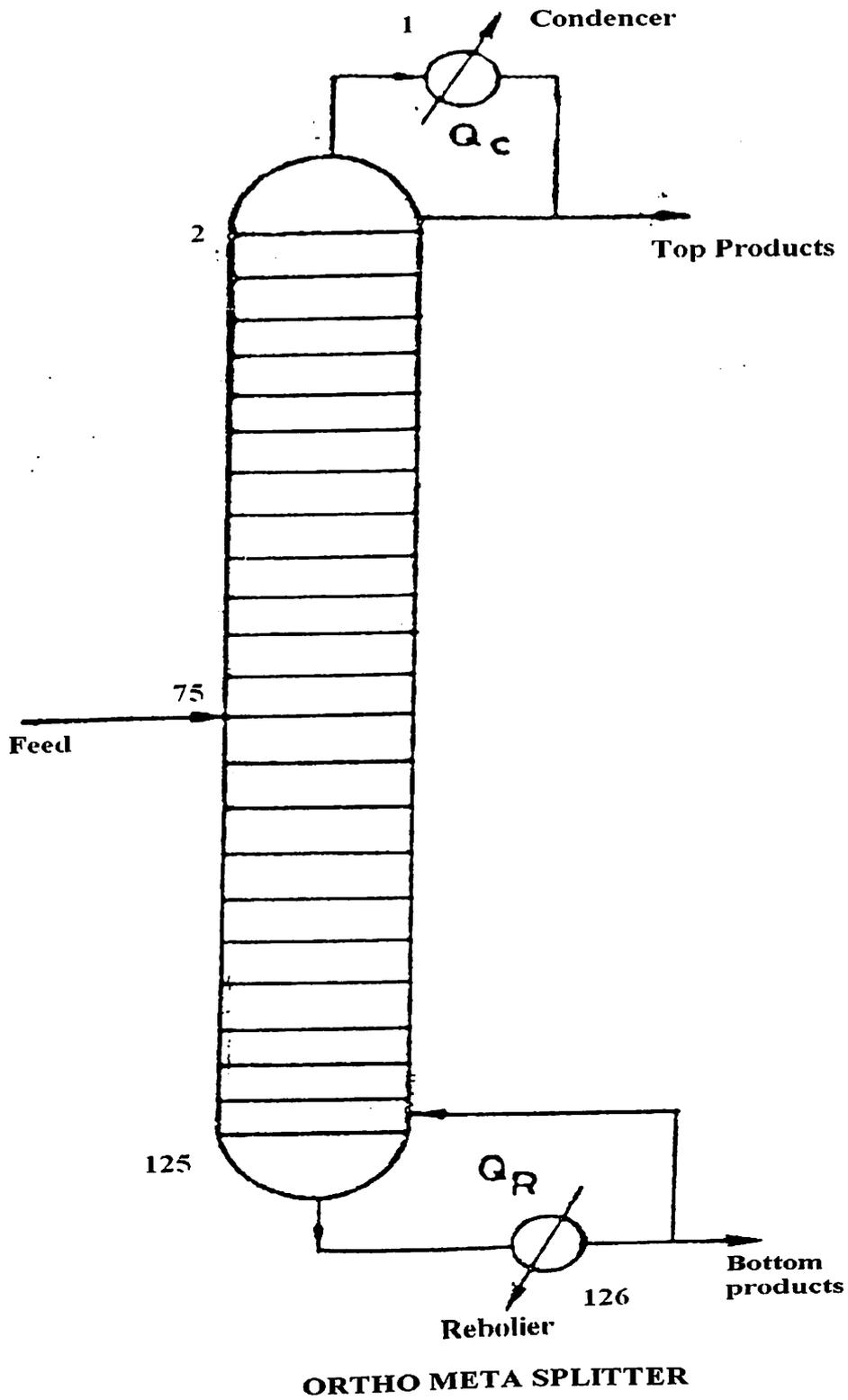
(Fig 1)

(Schematic diagram of Ortho Meta Splitter)

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1.1 <u>Literature Review</u>

OMS is a simple, multi-stage, multi-component, continuous distillation columns. In multi-stage, multi-component distillation column two types of problem arises, namely- Design and Simulation. (In design case column performance is given in terms of composition and we have to find out the critical number of equilibrium stages, feed plate, optimum reflux ratio etc. For solving design problems, very few method are available in literature). In case of simulation also know as rating problem is applicable to existing column. In this case the number of theoretical stages, feed plate location, reflux ratio etc., are known and composition of the products are required to be found out. For solving simulation, numerous number of methods are available in literature.

Here we concentrate only on simulation problem. This simulation comes under rigorous calculation. Rigorous is used for solving the fundamental equation allocated with multicomponent stage-wise separation like material balance, energy balance, equilibrium relation for each stage. All the co-relation and non-linear algebraic equation for solving these equations are quite tedious and iterative. The accuracy depends upon phase equilibrium and enthalpy data utilized. Once program has developed, it is easy to get desired solution.

In this thesis work, we are using Naphtha and Sandholm (1971) procedure for solving distillation problem; all the material balance, energy balance, equilibrium relations are grouped stage wise and then linearized. The resulting set of equations has block tri-diagonal structure, which gives solution by simple technique. T_i, L_{ij} and V_{ij} are taken as independent variables and simultaneous connection (SC) procedure is used for new set of variables. This method can handle various types of separation problems. The advantage of this method is, it can handle non-ideal thermodynamics and murphree plate efficiencies in a rigorous manner. It is flexible in specification, can use multiple feeds, no difficulties of rounding of errors. The disadvantage of this method is its requirement of large computer storage space and initial guesses.

1.2 Process Description

Fractionation unit:

The Xylene fractionation unit, process the deheptanised C_8+ isomerisate from isomerisation unit and C_8+ reformate from reformer unit to make it unsaturated free. Then the two streams are sent to the Ortho-meta splitter column. The top product consists of Para-Xylene, ethyl benzene, Meta-Xylene, which is sent to the Parex Unit. The bottom product is C_9 Aromatics quantities along with desired quantities of O-Xylene.

Description:

The deheptanised C_8+ reformate received from Reformer Plant, is preheated with outgoing clay treated reformate in the tube side of the exchanger and then by hot oil is fed to the Clay treaters. The basic function of the Clay treater is to remove any unsaturated present in the feed stock formed during the reforming operation.

Similarly C_8+ isomerisate, received from Isomerisation Unit is preheated in feed effluent exchanger or outgoing clay treated isomerisate in the tube side of the exchanger and then by hot oil, is fed to the Clay treater. The clay treaters operate at a pressure of 12 kg/cm^2 and 175° C. The two streams of is continuously pumped into Ortho-meta splitter. This column operates at a pressure of 105 kg/cm^2 and top temperature of 156° C and bottom -186° C. The function of Ortho-meta splitter is to remove all C_9 Aromatics along with desired O-xylene from the feed. The top product of Ortho-meta splitter is Para-Xylene + Meta-Xylene +Ortho Xylene+ Ethyl Benzene A portion of it, is pumped back to the column as reflux while the remaining hot product at 145°C is sent directly as feed stock to Parex Unit. The bottom product is Ortho-xylene + C_9, which is heated in a stream heated kettle type reboiler due to which it is partly vaporized. It is the returned to column, while Ortho-xylene bearing liquid is fed to Ortho-rerun column.

SHORT- CUT METHOD

2.1 Introduction to Short-cut:

Short-cut method is the quick hand calculation method for multicomponent, multistage, continuous distillation column. The following steps are involved for calculations of different parameter by Short-cut method.

STEP1: Guess light key & heavy key component.

STEP2: Shiras equation for find out distributed &undistributed components

STEP3: Use Underwood equation to find minimum reflux.

STEP4: Use Fenske equation for finding minimum number of trays at total reflux.

STEP5: Gilland Co-relation to find number of trays.

STEP6: Use Drickamen & Brend to find approximate tray efficiency by knowing Viscosity of feed.

2.2 Material balance:

Table 1.(Feed & Product composition (Wt %) From"BRPL")

Basis of the calculation is taken as 1 hour

Feed flow rate is 29,111 kg/hr from Material Balance

Components	Feed of OMS (wt %)	Top distillate of OMS (wt %)	Bottom of OMS (wt %)
Saturate, C_8, C_9	2.37	2.48	Nil
Toluene	0.04	0.09	Nil
Ethyl Benzene	20.5	21.63	Nil
P – Xylene	15.22	16.06	Nil
M – Xylene	41.96	42.98	0.12
O – Xylene	18.92	17.03	41.12
C_9^+ Aromatics	0.99	Nil	58.96
Total	100.00	100.00	100.00

Table 2. (Conversion Wt% in to mole % of feed and products)

Basis of calculation is taken as 1 hour

Feed flow rate is 29,111 kg/hr from Material Balance

Components	Feed OMS (wt %)	Feed flow rate x wt% = in kg	Molecular wt in kg	No. of Moles	Mole %
Saturate	2.37	684.9	128	5.28	2.3
Toluene	0.04	11.6	92	0.13	Negligible
Ethyl Benzene	20.5	5967.7	106	56.29	20.7
P – Xylene	15.22	4436.6	106	41.79	15.31
M – Xylene	41.96	12214.91	106	115.3	42.25
O – Xylene	18.92	5507.8	106	51.96	19.04
C_9^+ Aromatics	0.99	288.2	120	2.12	0.8
Total	100 %	29,111		272.8	100 %

Table 3 (Conversion Wt% in to mole % of top products)

Basis of calculation is 1 hour

Distillate flow rate is 27,333 kg/hr

Components	OMS distillate (wt%)	Distillate flow rate x wt% =in kg	Molecular wt in kg	No. of moles	Mole %
Saturate (C_9)	2.48	617.85	128	5.28	2.03
Toluene	0.09	24.5	92	0.266	Negligible
Ethyl benzene	21.63	5912.12	106	55.77	21.61
P – Xylene	16.06	4389.6	106	41.41	16.03
M – Xylene	42.98	11747.72	106	110.91	43.17
O – Xylene	17.03	4654.8	106	43.91	17.16
C_9^+ aromatics	Nil	Nil	Nil	Nil	Nil
Total	100 %	27,333		257.28	100 %

Table 4. (Conversion Wt% in to mole % of bottom products)

Basis of calculation is 1 hour

Bottom flow rate is 1778 kg/hr

Only meta-xylene, ortho-xylene and C_9^+ are present, remaining are absent

Components	OMS bottom wt%	Feed x wt% = in kg	Molecular wt in kg	No. of moles	Mole %
M – Xylene	0.12	2.13	106	0.02	0.12
O – Xylene	41.12	731.11	106	6.89	44.11
C_9^+ Aromatics	58.76	1044.75	120	8.71	55.77
Total	100 %	1777.99		15.62	100 %

2.3 Thermodynamics:

2.3.1 Table 5. (Vapor ressure at different temperature.) (3)

Components	10 mm Hg	20 mm Hg	40 mm Hg	60 mm Hg	100 mm Hg	200 mm Hg	400 mm Hg	760 mm Hg
Saturate (C_9)	38°C	51.2^{O}C	66°C	75.5^{O}C	88.1^{O}C	107.5^{O}C	128.2^{O}C	150.8^{O}C
Toluene	6.4	18.4	31.8	40.3	51.9	69.5	89.5	110.6
E-Benzene	25.9	38.6	52.8	61.8	74.1	92.7	113.8	136.2
O-Xylene	32.1	45.1	59.5	68.8	81.3	100.2	121.7	144.4
M-Xylene	28.3	41.1	55.3	64.4	76.8	95.5	116.7	139.1
P-Xylene	27.3	40.1	54.4	63.5	75.9	94.6	115.9	138.3
C_9^+Aromatics	55.9	69.9	85.4	95.3	108.8	129	152	176.1

Above table gives temperature according to pressure. To make it simplification by interpolating, I calculate the pressure according to temperature and then logarithm of pressure. Below the table gives to logarithm of vapor pressure at different temperature.

Table 6. (logarithm of vapor pressure at different temperature)

Log of vapor pressure	40 ^{O}C	60 ^{O}C	80 ^{O}C	100 ^{O}C	120 ^{O}C	140 ^{O}C
Saturate	1.056	1.5	1.867	2.2	2.5	2.76
Toluene	1.778	2.16	2.48	2.76	3.0	3.23
E-Benzene	1.343	1.744	2.11	2.42	2.7	2.93
P & M-Xylene	1.295	1.7	2.06	2.38	2.65	2.92
O-Xylene	1.203	1.6	1.98	2.3	2.58	2.84
C_9^+ Aromatics	0.658	1.11	1.51	1.86	2.2	2.47

As Para and meta Xylene have close boiling point, so the vapor pressure at different temperature are approximately identical. Hence I have taken Para and meta Xylene are same value of vapor pressure.

The feed temperature of OMS is 175 $^{\circ}$C. Due to non-availability of vapor pressure at 175 $^{\circ}$C in Hand book of Chemical Engineering by Perry. According to Ref: 3, Plot a graph log vapor pressure vs temperature and extend the line, so that we will get the vapor pressure at 160 $^{\circ}$C and 175 $^{\circ}$C.

2.3.2 Distribution co-efficient

Distribution co-efficient is denoted by k or m.

$$k = \frac{\text{Vapor pressure of j}^{th}\text{ component}}{\text{Total pressure}} = P_j / P_t$$

In OMS total pressure is 1 atmosphere = 760 mm Hg

Table 7. Distribution Coefficient (k)

k value	40 $^{\circ}$C	60 $^{\circ}$C	80 $^{\circ}$C	100 $^{\circ}$C	120 $^{\circ}$C	140 $^{\circ}$C	160 $^{\circ}$C	175 $^{\circ}$C
Saturate	0.015	0.041	0.0977	0.212	0.422	0.773	1.76	3.12
Toluene	0.079	0.192	0.401	0.76	1.36	2.25	7.4	13.03
E-Benzene	0.029	0.073	0.173	0.35	0.657	1.14	2.78	4.94
P&M Xylene	0.0263	0.066	0.154	0.319	0.596	1.11	2.34	4.16
O-Xylene	0.0211	0.051	0.126	0.262	0.505	0.91	2.08	3.7
C$_9^+$Aromatics	0.006	0.017	0.043	0.097	0.204	0.39	0.434	1.476

2.3.3 Flash vaporization of feed (1)

This implies how much liquid to vapor ratio at flash zone. First we assume how much vapor and liquid. Substitute all the value in the equation

$$y_{jD} = \frac{Z_{jf}(L/G +1)}{1 + (L/G)k}$$

If the value of $\sum y$ = 1, then our assumption is right or else take another assumption and find $\sum y$. After several trials, assume G_f = 0.99 and L_f = 0.01. feed (f) = 1.

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L/G = 0.01/0.99 = 0.01. at 175 °C almost all the feed in gaseous state and little amount in liquid state.

Table 8.(Flash Vaporization)

Components	Feed mole fraction (Z_f)	k_{175}	Y_{jD}
Saturate	0.023	3.12	0.025
Toluene	Negligible	13.03	Negligible
Ethyl Benzene	0.207	4.94	0.2
P & M Xylene	0.5756	4.16	0.56
O – Xylene	0.1904	3.7	0.19
C_9^+ Aromatics	0.008	1.476	0.01
Total			0.985=1

2.4 Problem formulation:

2.4.1 Key Components (1)

It is convenient first to list the feed components in order of their relative volatility. The more volatile components are called light, the less volatile are called heavy. We should choose one light key component such that it should present important amount in distillate and little amount in bottom. Similarly, heavy key component also present in both the stream lighter than the light key component present in bottom of the OMS.

If all components are found in the distillate, then choose the least volatile as heavy key component.

For multi component system, Relative volatility (α) of jth component is $\alpha_j = k_j / k_{hk}$

k_j = distribution co-efficient of jth component

k_{hk} = distribution co-efficient of heavy component

According to above definition $\alpha_{hk} = 1$ always

2.4.2 Table 9 (Relative Volatility HK & LK)

Components	Mole fraction of feed (Z_f x f)	k_{175}	α_{175}
Saturate	0.023	3.12	0.843
Ethyl Benzene	0.207	4.94	1.33
P-Xylene	0.1531	4.17	1.124
M-Xylene	0.4225	4.17	1.124
O-Xylene	0.1904	3.7	1.0
C_9^+ Aromatics	0.008	1.476	0.398

2.4.3 Distributed & Un Distributed Components (: 1)

To find distributed and undistributed components, one empirical co-relation is given as:

$$\frac{y_{jD}\,D}{Z_{jF}\,F} = \frac{\alpha_j - 1}{\alpha_{lk} - 1} \times \frac{y_{lkD}\,D}{Z_{lkf}\,F} + \frac{\alpha_{lk} - \alpha_J}{\alpha_{lk} - 1} \times \frac{X_{hkD}\,D}{Z_{hkf}\,F}$$

If $(y_{jD}D/Z_{jF}F)$ values come less than -0.01 or greater than 1.01, components j will probably not distribute. For $(y_{jD}D/Z_{jF}F)$ values lies between 0.01 and 0.99, component j will undoubtedly distribute.

$$y_{lkD}\,D = 0.4225 \times 0.431 = 0.1821$$

$$y_{hkD}\,D = 0.1904 \times 0.17 = 0.0325$$

For Saturate:

$$\frac{y_{jD}\,D}{Z_{jF}\,F} = \frac{0.843 - 1}{1.124 - 1} \times \frac{0.1821}{0.4225} + \frac{1.124 - 0.843}{1.124 - 1} \times \frac{0.0325}{0.1904} = -0.158$$

For Ethyl Benzene:

$$\frac{y_{jD}\,D}{Z_{jF}\,F} = \frac{1.33 - 1}{1.124 - 1} \times \frac{0.1821}{0.4225} + \frac{1.124 - 1.33}{1.124 - 1} \times \frac{0.0325}{0.1904} = 0.863$$

For Para Xylene:

$$\frac{y_{jD}\,D}{Z_{jF}\,F} = \frac{1.124 - 1}{1.124 - 1} \times \frac{0.1821}{0.4225} + \frac{1.124 - 1.124}{1.124 - 1} \times \frac{0.0325}{0.1904} = 0.431$$

For Meta Xylene:

$$\frac{y_{jD}\,D}{Z_{jF}\,F} = \frac{1.124 - 1}{1.124 - 1} \times \frac{0.1821}{0.4225} + \frac{1.124 - 1.124}{1.124 - 1} \times \frac{0.0325}{0.1904} = 0.431$$

For Ortho Xylene:

$$\frac{y_{jD}\,D}{Z_{jF}\,F} = \frac{1 - 1}{1.124 - 1} \times \frac{0.1821}{0.4225} + \frac{1.124 - 1}{1.124 - 1} \times \frac{0.0325}{0.1904} = 0.1707$$

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<u>For C_9^+ Aromatics:</u>

$$\frac{y_{jD}\ D}{Z_{jF}\ F} = \frac{0.38 - 1}{1.124 - 1} \times \frac{0.1821}{0.4225} + \frac{1.124 - 0.398}{1.124 - 1} \times \frac{0.0325}{0.1904} = -1.1308$$

From the above calculation saturate and C_9^+ aromatics are undistributed. Light key and heavy key components are always distributed and here ethyl benzene also distributed.

2.5 Calculation of Minimum Reflux (1)

By Underwood's method, which uses constant average value of relative volatility and assume constant L/G, is not exact but provides reasonable values without great effort.

For finding out minimum Reflux (R_m), two equations must be solved.

1. $\sum \{(\alpha_j\ Z_{jF}\ F) / (\alpha_s - \Phi)\} = F\ (1-q)$

2. $\sum \{(\alpha_j\ x_{jD}\ D) / (\alpha_j - \Phi)\} = D\ (R_m + 1)$

$q = L_f / F = (0.01/1) = 0.01$

<u>Value of Φ:</u>

$\sum \{(\alpha_j\ Z_{jF}\ F) / (\alpha_s - \Phi)\} = F\ (1-q)$

This Φ value must lie between the relative volatility of light and heavy key component. After several trials the value of Φ, I have found out to be approximately 1.03.

Substitute this Φ value in second equation:

$\sum \{(\alpha_j\ x_{jD}\ D) / (\alpha_j - \Phi)\} = D\ (R_m + 1)$

Since saturate, Ethyl Benzene, Ortho Xylene are absent in bottom, so there component whatever in feed, directly goes to distillate. So feed mole % is equal to distillate. No C_9^+ Aromatics in top, so leave this term.

But Meta Xylene and Ortho Xylene are both the stream, so I should multiply the % of distillate.

$$D\ (R_m + 1) = 3.742$$

How much amount of saturate, Ethyl Benzene and Para Xylene present in feed, same amount in distillate. But meta Xylene in feed 115.23 moles and distillate 110.91.

So, Meta Xylene % of recovery = (110.91/115.23) x 100 = 96 %

In mole % 0.4225 x 96 = 0.4056 = 0.017

Similarly Ortho Xylene in top is 17.16%

Hence Ortho Xylene in top = 0.1904 x 0.1716 = 0.032

and in bottom = 0.1904 – 0.032 = 0.157

Table 10. (Total distillate & bottom products)

Components	y_D D	x_W W
Saturate	0.023	Nil
Ethyl Benzene	0.207	Nil
Para Xylene	0.1531	Nil
Meta Xylene	0.4056	0.017
Ortho Xylene	0.032	0.157
C_9^+ Aromatics	Nil	0.008
	D = 0.821	W = 0.179

$D (R_m + 1) = 3.742$

$(R_m + 1) = (3.742 / 0.82) = 4.56$

$R_m = 4.56 – 1 = 3.56$

But in BRPL, actual Reflux ratio is 2.5

2.6 Bubble Point & Dew Point Calculation (5)

Bubble point is the initial boiling point of a liquid mixture.

Dew point is the initial condensation temperature.

Basic equation for bubble point and dew points are:

$\sum y_i = \sum k_i x_i = 1.0$ (i = 1 to N_C)

$\sum x_i = \sum y_i / k_i = 1.0$ (i = 1 to N_C)

where N_C is the number of components.

First we have to assume a temperature. Value of distribution co-efficient (k_i) are found from graph and table.

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For bubble point, find the value of y_i. If summation of y_i is greater than 1, then choose less temperature and vice versa. When summation of y_i is equal to 1, then our assumption is right. Similarly, for dew point, if summation of x_i is less than 1, then choose less temperature and vice versa. When we will get summation x_i is equal to 1 then our assumption is right.

By several Trial, I found a temperature at $135^{\circ}C$, which is approximately equal to 1. Since boiling point of Ortho, meta & Para Xylene and ethyl benzene are close enough, so bubble point & dew point are slightly varying.

Table 11.(Bubble Point & Dew Point)

Components	x_i or y_i	P_i in mm Hg @ $135^{\circ}C$	$k_i = P_i / 760$	$y_i = k_i x_i$	$x_i = y_i / k$
Saturate	0.023	530.8	0.698	0.016	0.032
Ethyl benzene	0.207	841.0	1.10	0.227	0.188
P-xylene	0.1531	668.3	0.88	0.1425	0.134
M-xylene	0.4225	668.3	0.88	0.393	0.372
O-xylene	0.1904	630.9	0.83	0.158	0.223
C_9^+Aromatics	0.008	266.0	0.35	0.002	0.022

$$\Sigma y_i = 0.9385 \qquad \Sigma x_i = 0.971$$

By interpolating & extrapolating, I found BP = $133^{\circ}C$ & DP = $137^{\circ}C$

2.7 Theoretical Trays (1)

Fenske's equation is applied both binary and multicomponent system for calculation of theoretical trays.

$N_m + 1 = \{\log[(x_{lk}D / x_{hk}d) (x_{hk}W / x_{lk}W)]\} / (\log \alpha_{lk} \text{ avg})$

Where $N_m + 1$ = Total number of theoretical trays including reboil and partial condenser

α_{lk} avg = $(\alpha_{lk \text{ bubble point}} \times \alpha_{lk \text{ dew point}})^{0.5}$

Since bubble point is $133^{\circ}C$ and dew point is $137^{\circ}C$

α_{lk} avg = $135^{\circ}C$, at $135^{\circ}C$ vapor pressure light key = 668.34 mm Hg (from graph)

Total pressure = 760 mm Hg

Similarly,

k_{lk} = 668.34 / 760 = 0.88

k_{hk} = 630.9 / 760 = 0.83

α_{lk} = k_{lk} / k_{hk} = 1.06

N_m + 1 = {log[(0.4056 / 0.032) (0.157 / 0.017)]} / log 1.06 = 2.068/0.25

= 82.73

N_m = Total no. of theoretical trays without reboiler

N_m = 81.73

2.8 Tray Efficiency & Total Efficiency: (4 & 2)

Since I do not have the data of x & y at each stage, I am unable to find Murphy efficiency & total efficiency.

But Drickamen and Brend Ford have given one empirical co-relation and find out approximate efficiency to obtain some idea of possible stages. This empirical co-relation & graph is approved by American Institute of Chemical Engineer's distillation tray efficiency research.

This method is used to find out the viscosity of each component and multiplied by mole fraction present in feed and take the summation. After getting summation compare with the graph and find out the total efficiency.

Table 12. (Total Viscosity)

Components	Mole fraction in feed	Viscosity calculation X	Viscosity calculation Y	$\mu_i C_p$	$\mu_i x_i$
Saturate	0.023	13.7	10.0	0.14	0.003
Ethyl Benzene	0.207	13.2	11.5	0.17	0.035
P-xylene	0.1531	13.9	10.9	0.165	0.025
M-xylene	0.4225	13.9	10.6	0.16	0.067
O-xylene	0.1904	13.5	12.1	0.20	0.038
C_9^+Aromatics	0.008	12.5	10.9	0.12	0.001

$\sum \mu_i x_i = 0.17$

From graph at 0.17, total efficiency is 65%

Actual no. of trays = Theoretical trays / Total efficiency = 81.73 / 0.65 = 125.73

Approximately 126 trays.

2.9 Other specification:

Total number of trays=126

Feed tray location in OMS has three option

Feed tray number 75 – For production of 6000 MTPA of O-xylene

Feed tray number 79 – For production of 7200 MTPA of O-xylene

Feed tray number 69 – This tray is used when the feed contain more C_9^+ Aromatics

Feed temperature is 175 ^{O}C.

Top and bottom of OMS temperature are 156 ^{O}C and 186 ^{O}C respectively.

These trays are valve type trays.

Trays are two passes throughout the column.

These valve trays number is SS410.

We used the kettle type reboiler.

Length of OMS column = 49.3 meters

Diameter of OMS column = 3.6 meters

Tray spacing between two trays = 350mm

Continuous online analyzer provide for checking of C_9^+ Aromatics in OMS reflux stream.

OMS column is made up of Carbon Steel

Trays are also made up of Carbon Steel

RIGOROUS METHOD

3.1 Development of Mathematical :

Ortho-meta splitter (OMS) is a simple column, because it has one feed, a top product, a bottom product and no side products. The column can have top condenser or reboiler and bottom reboiler, but no inter-reboiler or inter-condenser. This column follows the Rigorous method as a group of equation and solves these equations to calculate the operating condition of the column. When a rigorous calculation is performed, the followings are usually specified:

1. Rate, composition and condition of end feed
2. Number of stages in column
3. Separation specification
4. Column pressure profile

Column design and performance calculation present the column at steady state. What enters the column matches with what exits.

$\sum$ (Molar feed flow rate) = $\sum$ (Molar Product flow rate)

$\sum$ (Moles of any component in feed) = $\sum$ (Moles of component in the product)

Feed enthalpy + heat added = Product enthalpy + heat removed

3.1.1 MESH Equation:

MESH equation is used to describe the steady state operation of a distillation column. MESH stands for

Material Balance Equation, both component and total

Equilibrium equation, including bubble point and dew point equation

Summation of Stoichometry equations

Heat or enthalpy or energy balance equations

These equations define the overall column Material Balance, Energy Balance and Product composition. Internal to the column, they describe equilibrium conditions, internal (stage – stage) component, total material balance and

internal energy balance. The independent variables of a column are the product rates and composition, internal vapor and liquid rates, composition and stage temperature. Equilibrium constant, K-values and mixture enthalpies are dependent variables. Each stage is assumed to be an equilibrium stage. This rigorous method, thus convert a column to a group of variables and equations. The equations are first referred to as a MESH equation. This MESH variable are often referred as state variable such as

- Stage temperature, T_j
- Internal total vapor and liquid rates, V_j and L_j
- Stage composition, y_{ij} and x_{ij} or component vapor and liquid rates V_{ij} and L_{ij}

3.1.2 Naphthali – Sandholm method:

This method choose the stage temperature and component vapor and liquid rate from the MESH variable of the Newton-Raphson calculation. The MESH equation serving has independent functions and grouped by stage are the energy balance, a component balance for each component and equilibrium equation for each component. These are $(2C + 1)$ equation for stage and with $N(2C + 1)$ equations for full column.

l_{ij} - Molar flow rate of component i, leaving j^{th} tray in liquid phase

v_{ij} – Molar flow rate of component i, leaving j^{th} tray in vapor phase

V_j – Total flow rate of vapor and liquid leaving j^{th} tray

j – No. of trays $j - 1, 2 \ldots \ldots 126$

i – Components $i - 1, 2 \ldots \ldots .7$

H_j, h_j – Molar enthalpy of vapor and liquid streams leaving the stage

$f^L_{i,j}, f^V_{i,j}$ – Molar flow rate of jth component in the feed entering the ith tray

Number of independent variables l_{ij}, v_{ij}, T_j

3.1.3 General Tray equations:

Mass balance:

$$M_{i,j} = l_{i,j-1} + V_{i,j-1} - l_{i,j} - v_{i,j} + f^{L}_{i,j} + f^{V}_{i,j}$$

$$\text{Where } j - 1,2.......7$$

$$i - 2,3.......126$$

M_{ij} =Discrepancy factor, which is assigned a value at the start of simulation and will be close to zero at the end of simulation.

Equilibrium:

$$y_{i,j} = K_{i,j} * x_{i,j} \quad (\eta_{i,j} = 1)$$

$$\text{Where} \quad j - 1,2........7$$

$$i - 2,3.......126$$

$$y_{i,j} = v_{i,j} / \Sigma \, v_{i,j} \quad \text{and} \quad X_{i,j} = l_{i,j} / \Sigma \, l_{i,j}$$

Enthalpy Balance:

$$H_i = L_{i-1,} * h_{i-1} + V_{i+1} * H_{i+1} - L_i * h_i - V_i * H_i + f_i^{L} * h_i^{F} + f_i^{V} * H_i^{F} - Q_i = 0$$

$$\text{Where,} \quad j - 1,2......7$$

$$i - 1,2......126$$

3.1.4 Total Condenser:

Component balance:

$$M_{1,j} = v_{2,j} - v_{1j} - l_{1,j} = 0$$

$$\text{Where,} \qquad j - 1,2......7$$

Equilibrium relations:

$$E_{1,j} = (v_{1,j} / V_1) - (l_{1,j} / L_1)$$

$$\text{Where,} \quad j - 1,2......7$$

Specification equations:

$$H_{1R} = L_1 - RV_1$$

Where $R = L_1 / V_1$

3.1.5 Partial Reboiler:

Component material balance:

$$M_{126} = I_{125\,j} - V_{126,\,j} - I_{126,\,j}$$

Where,   j-1...13

Equilibrium balance:

$$V_{126,\,j} = K_{126,\,j} * L_{126,\,j}$$

Where,   j-1.2.....7

Enthalpy balance:

$$H_{126} = L_{126} - L_{126}{}^{S}$$

Where, $L_N{}^{S}$ = Total bottom product withdrawn

These mathematical model equations can be solved in an iterative process to improve upon such that results match the real system. They are conceptual and in dimensionless form which can be solved by using mathematical software's like Matlab, Mathmatica.

3.2 Simulation by Aspen Hysys:

Aspen HYSYS is a software solution for the process industry. This is the basic concept necessary for creating simulation in Aspen HYSYS. Hysys gives direction how to determine properties of these streams by using the phase and the property table utilities.

1. Define fluid package (property package, library components, hypothetical components)
2. Add streams
3. Understand flash calculations
4. Attach stream utilities
5. Customize the work book

3.2.1 Simulation Basis Manager:

HYSYS uses the concept of fluid package to contain all necessary information for performing flash and physical property calculations. This approach allows us to define all information (property package, components, hypothetical components, interaction parameters, reactants, tubular data, etc.) inside a single entity.

1. All associated information is defined in a single location, allowing for easy creation and modification of information.
2. Fluid packages can be stored as completely defined entities for use in any simulation.
3. Components list can be stored out separately from the fluid package as completely defined entities for use in any simulation.
4. Multiple fluid packages can be used in the same simulation.

The simulation basis manager is a property view that allows us to create and manipulate multiple fluid package or component lists in simulation.

3.2.2 Steps involved in Simulation by Aspen HYSYS:

1. Start a new case by selecting the new case icon.
2. Create a fluid package by clicking the add button.
3. Choose the fluid package (Peng-Robinson Equation)
4. Adding the component list by clicking view button.
5. Select the hypothetical menu item in the add components box to add a hypothetical components in the fluid package. A hypothetical component can be used to model non-library components of defined or undefined mixtures. Hypothetical component is used to model the components heavier than that component.
6. When hypothetical component has been defined, return to the fluid package and add the hypothetical component in the selected component.

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7. Adding material streams:- In HYSYS, there are two types of streams such as material and energy. Material streams have a composition and parameter such as temperature, pressure and flow rate. These represent the process stream

8. Adding the Unit Operation to OMS:

    The OMS column is modeled as a multi-component, multi-stage, simple distillation column with 126 stages, 125 trays in the column plus the reboiler and total condenser. It operates at a pressure of 1.5 atm. The objective of the column is to produce a 100% of C_9+ aromatics in the column.

9. Click on the distillation column bottom and enter the necessary information. After entering click the run button to run the column. Number of iteration we specified as 10,000. Once the column has converged, then check the product quality or else go to the ∵

10. Once the system has converged, then compare the product quality we are getting from HYSYS and actual data from industry. If product quality are varying then changed the assign parameters.

3.2.3 Flash Calculation:

Once the composition of the stream and two of either temperature, pressure or vapor fraction are known. HYSYS performs a flash calculation on the stream calculating the third parameter.

Note: If we give temperature, pressure and vapor fraction, a consistency error will come with the flash capabilities of HYSYS. It is possible to perform dew and bubble point calculations. By specifying a vapor fraction of 1.0 and either the pressure or temperature of the stream, HYSYS will calculate the dew temperature or pressure. To calculate bubble temperature or pressure, a vapor fraction of 0.0 and either pressure or temperature must be entered.

3.2.4 Design Case:

The feed composition has taken from Chemical Laboratory at BRPL. All the composition has analyzed by G.C analysis. The composition are follows

Table 13. (Feed Wt fraction)

Feed	Wt fraction
n Nonane	0.0214
Toluene	0.0045
E-Benzene	0.1551
P-Xylene	0.1572
M-Xylene	0.4221
O-Xylene	0.1996
C9+ Aromatics	0.0400

The mass flow rate of feed to OMS is 29111kg/hr. The amount of C9+ Aromatics present in feed has been recovered by 99.65% at bottom of the OMS. Under this high recovery of C9+ Aromatics condition, we maximized O-Xylene recovery at the bottom of the OMS

3.2.5 Simulation Results for Design Case:.

The simulation process was done using Aspen Hysys version 2004 and the results obtained are as follows:

OMS splitter:

The specifications under which the splitter was converged:

a) C9+ Aromatics recovery   99.65 %

b) Reflux flow rate   68333.7 kg/hr

The specification should be selected such that the degree of freedom is zero, which is a basic condition for simulation process.

Table 14. (Material balance design case OMS splitter)

Mass flow rate to OMS is 29111 Kg/hr .

Parameter	Value
Reflux drum Pressure	101.3 KPa
Reflux drum Temperature	139.1C
Column top pressure	103.3 KPa
Column top temperature	140.1 C
Column bottom pressure	202.6 KPa
Column bottom temperature	181.2 C
Reboiler O/L temperature	183.1 C
Reflux flow rate	68333.7 kg/hr

Table 15.Product composition and rates (Composition in Wt fraction basis)

Component	Calculated OMS Top(27333 Kg/hr)	Calculated OMS Btm (1778 Kg/hr)
n Nonane	2.27538217817745e-002	6.16683899415276e-004
Toluene	4.79311503538776e-003	5.47239341628655e-020
E-Benzene	0.165200424826349	3.49590608112562e-005
P-Xylene	0.167374629571247	9.97316692789903e-004
M-Xylene	0.449363200626435	3.55203939021116e-003
O-Xylene	0.190514808158783	0.339634283298224
C9+ Aromatics	2.28963819957105e-014	0.655164717658548

Table 16.Simulation output expected:

Condenser Duty	3.26796 e+007 kg/hr
Reboiler Duty	3.056 e+007 kg/hr
Bottom Column Pressure	202.6 KPa
Overhead Product rate	27333 kg/hr

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3.3 Thermodynamic properties:

3.3.1 Comparisons of different thermodynamics properties

The vapor-liquid equilibrium ratio i.e. K-values and the enthalpy are the two important thermodynamic properties required for distillation problems. Graphical representation of thermodynamic properties is not convenient to use for multicomponent distillation calculations. For ease of computations, these properties should be expressed in terms of simple algebraic equations. However, since mixture properties depend on temperature, pressure, and phase compositions, these equations tend to be complex.

As the design and simulation calculations are quite sensitive to thermodynamic properties, a particular method of calculation cannot be expected to handle all types of mixtures with the same degree of accuracy. The method to be selected greatly depends on the extent of non ideality of the mixture. For ideal mixtures, various types of analytical expressions are available. For vapor-liquid equilibrium to exist the fugacity of each component in the two phases are equal at a particular temperature and pressure.

$$f_j^L \equiv f_j^V, \ j = 1,2,\ldots\ldots C$$

To form an equilibrium ratio, fugacities are replaced by equivalent expressions involving mole fractions. Many replacements are possible from thermodynamic point of view, but the most commonly used one is

$$f_{jV} = \Phi_{jV} \ y_j \ P \text{ and } f_{jL} = \Phi_{jL} \ x_j \ P$$

where Φ_{jV} and Φ_{jL} are the fugacity coefficients in vapor and liquid phases respectively which account for the non ideality of the phases.

Therefore,

$$K_j = y_j/x_j = \Phi_{jL}/ \Phi_{jV}$$

3.3.2 Thermodynamic Properties for Non-ideal solution:

For calculation of Φ_{jL} and Φ_{jV}, equation of state can be used and the accuracy depends on the PVT relation used. For distillation calculations, cubic equations of state, but the most commonly used are Soave-Redlich-Kwong (SRK) ,Peng-Robinson (PR), Braun K10 (BK10) equations. These equations apply to both vapor as well as liquid phases. These are two parameter equations of state and use pure component properties. For highly polar molecules, these are not applicable for liquid phase fugacity coefficient calculations. For those cases UNIFAC model is commonly used. . Here we discuss these four methods for thermodynamic properties estimation.

This table shows , how the duties, pressure and products rate have changed by changing different thermodynamics properties.

Table 17. (Comparison of different thermodynamics properties.)

	Desired output	Peng Robinson	BK 10	PR-TWU	SRK-TWU
Condenser Duty, 10^7 kg/hr	3.2681	3.26796	3.25747	3.25714	3.26208
Reboiler Duty, 10^7 Kg/hr	3.045	3.056	3.023	3.039	3.045
Bottom Pressure, KPa	202.1	202.6	202.5	202.6	202.5
Overhead Product rate, kg/hr	27333.33	27333	27333	27332.92	27333
Bottom Product rate, kg/hr	1777.77	1778	1777.98	1778.3	1778.2

From the above comparison , Peng Robinson thermodynamics properties are closely related to desired out put. Even though PR-TWU, SRK-TWU results are nearly close to our desired output. Hence we have used the Peng Robinson thermodynamics properties for further simulation and sensitivity analysis.

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RESULTS AND DISCUSSION

The simulation result obtained from Aspen HYSYS 2004 version and the resulting analysis has been studied under different condition. Following flexibilities are available with respect to column simulation and operation.

(i)   Total condenser

(ii) One feed stream

(iii) Number of side stream

(iv) Non-ideal thermodynamic system

(v)   Specification and Operating conditions

All these consideration have been taken into account in the sensitivity analysis. In addition to computational calculation, the mathematical model has done by Naphthali-Sandholm method.

For thermodynamic properties calculation for non-ideal mixtures, we use from industrially useful practical methods:

(i)   Peng-Robinson

(ii) Soave-Redlich-Kwong-TWU

(iii) Braun K 10

(iv) PR – TWU

These four property estimation methods can take care of almost all practical multi-component distillation column.

4.1 Sensitivity Study:

Sensitivity analysis signifies ,how the product qualities changed by changing the parameter once at a time and other parameter remains unchanged.

4.1.1 Table 18. (Design case)

The Objective of OMS is to recover maximum amount of C_9^+ aromatics present in feed. The composition and recovery for the original design case are as follows:

D=27333,B=1778, F=29111kg/hr,R=2.5				
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS(Wt fraction)	Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.27E-02	2.43E-03	99.30982054	0.690179456
Toluene	4.79E-03	1.33E-21	100	1.81E-18
Ethyl Benzene	1.65E-01	2.93E-05	99.99884512	1.15E-03
P – Xylene	1.77E-01	1.31E-03	99.95201189	4.80E-02
M – Xylene	0.449327445	4.45E-03	99.9356844	6.43E-02
O – Xylene	0.181058334	4.02E-01	87.36783184	12.63216816
C_9^+ Aromatics	1.33E-05	5.89E-01	3.47E-02	99.96534041

These are the real feasible data has used an existing OMS at BRPL. In real practices we can recover 99.965% of C_9^+ Aromatics at bottom of the OMS. Under such condition we maximize O-xylene up to 12.7%. Other components are nearly same as practical data.

4.1.2 Table 19 . (Reflux ratio)

For reflux ratio 2.5, the composition and recoveries are follows:

R=2.5				
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)	Top distillate OMS (Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.27E-02	2.03E-03	9.94E+01	5.72E-01
Toluene	4.79E-03	1.29E-21	1.00E+02	1.73E-18
Ethyl Benzene	1.65E-01	2.80E-05	1.00E+02	1.09E-03
P – Xylene	1.77E-01	1.24E-03	1.00E+02	4.52E-02
M – Xylene	0.449120781	4.23E-03	99.93924202	6.08E-02
O – Xylene	0.181416116	3.99E-01	87.58387575	1.24E+01
C_9^+ Aromatics	1.33E-05	5.94E-01	3.47E-02	1.00E+02

if the reflux ratio is 2.5., we recover nearly cent percent of C_9^+ Aromatics and such condition theO-Xylene recovery is 12.4%. Other components are remaining unchanged.

Table 20, (Decreased Reflux ratio from 2.5 to 2.0.)

For decrease in reflux ratio from 2.5 to 2.0 composition and recoveries are follows :

R=2.0				
Components	Top distillate of OMS(Wt fraction)	Bottom of OMS (Wt fraction)	Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.24E-02	7.36E-03	9.79E+01	2.09E+00
Toluene	4.79E-03	2.59E-21	1.00E+02	3.51E-18
Ethyl Benzene	1.65E-01	5.47E-05	99.997848	2.15E-03
P – xylene	1.77E-01	2.37E-03	99.91314828	8.69E-02
M – xylene	0.449053149	7.94E-03	99.88537807	1.15E-01
O – xylene	0.181123996	4.02E-01	87.40888003	12.59111997
C_9^+ Aromatics	6.52E-04	5.80E-01	1.70E+00	98.29978848

If reflux ratio is decreased by 0.5 then there is a decrease in the recovery of C_9^+ Aromatics by 1.5%.but O-Xylene recovery remain same. Since the recovery of C_9^+ Aromatics percentage decreases, this condition has not recommended.

Table 21.Decreased Reflux ratio from 20 to 1.5:

For decrease in reflux ratio from 2.5 to 2.0 composition and recoveries are follows :

R=1.5				
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)	Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.11E-02	2.72E-02	9.23E+01	7.75E+00

Toluene	4.79E-03	2.13E-20		1.00E+02	2.90E-17
Ethyl Benzene	0.165153202	4.41E-04		99.98260309	1.74E-02
P – xylene	0.175971847	1.61E-02		99.40922097	5.91E-01
M – xylene	0.446240555	5.23E-02		99.24303723	7.57E-01
O – xylene	0.177983498	0.449519048		85.8788342	14.1211658
C_9^+ Aromatics	8.75E-03	0.4544758		2.28E+01	77.16827786

If reflux ratio is decreased by 0.5 then there is a decrease in the recovery of C_9^+ Aromatics by 21%.but O-Xylene recovery increase by 1.5%. Since the recovery of C_9^+ Aromatics percentage decreases largely , this condition never be used.

Table 22.Decreased Reflux ratio from 1.5 to 1.0:

For decrease in reflux ratio from 1.5 to 1.0 composition and recoveries are follows:

R=1.0					
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)		Top distillate of OMS(Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.10E-02	2.96E-02		9.16E+01	8.41E+00
Toluene	4.79E-03	4.72E-19		1.00E+02	6.40E-16
Ethyl Benzene	0.164790318	5.89E-03		99.76812177	2.32E-01
P – xylene	0.172164085	7.45E-02		97.2632328	2.74E+00
M – xylene	0.435586231	2.16E-01		96.87859172	3.12E+00
O – xylene	0.182640943	0.378138599		88.13069735	11.86930265
C_9^+ Aromatics	1.91E-02	0.2961897		4.97E+01	50.25158185

If reflux ratio further decreased by 0.5, then there is a decrease in the recovery of C_9^+ Aromatics by 27%.at the same time O-Xylene recovery also decrease by 2 %. Since the recovery of C_9^+ Aromatics percentage decreases steeply , this condition never be used.

Table 23.Increased Reflux ratio from 2.5 to 4.0:

For increase in reflux ratio from 2.5 to 4.0, the composition and recoveries are follows:

Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)		Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
R=4					
Saturate, C_8, C_9	2.28E-02	4.41E-04		9.99E+01	1.25E-01
Toulene	4.79E-03	4.80E-22		1.00E+02	6.51E-19
Ethyl Benzene	0.165174967	-		99.99952916	4.71E-04
P – xylene	0.17697419	5.66E-04		99.97920884	2.08E-02
M – xylene	0.449499021	1.97E-03		99.97146227	2.85E-02
O – xylene	0.180712783	0.407728676		87.19901166	12.80098834
C_9^+ Aromatics	1.12E-08	0.589280452		2.93E-05	99.99997071

By increasing reflux ratio from 2.5 to 3.0 ,3.0.to 3.5 and so on... we observed that there has no significant changed in recovery of C_9^+ Aromatics. Unnecessary increase in reflux ratio give more load to the column and the product has affected.

FLOW RATE:

4.1.3 Table 24. Increased feed flow rate by 10%:

For 10 % increase in feed flow rate from 29111kg/hr to 32022kg/hr, the composition and recovery are :

Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)		Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
10% increase in feed flow rate(32022 kg/hr)					
Saturate, C_8, C_9	2.27E-02	1.46E-03		9.96E+01	3.76E-01
Toulene	4.76E-03	8.66E-22		1.00E+02	1.07E-18
Ethyl Benzene	0.164199336	1.86E-05		99.99933274	6.67E-04
P – xylene	0.175916827	8.33E-04		99.97217124	2.78E-02

M – xylene	0.446805567	2.84E-03		99.96267044	3.73E-02
O – xylene	0.185645249	0.346615647		90.11114461	9.888855386
C_9^+ Aromatics	1.43E-05	0.648237416		3.74E-02	99.96260152

If the feed flow rate is increased by 10%, then the recovery of C_9^+ Aromatics remains same but the recovery of O-Xylene has decreased by 2.5%. increasing feed flow rate affect the product quality. Hence this condition may not applicable.

Table 25.Decreased feed flow rate by 10%:

For 10 % decrease in feed flow rate from 29111kg/hr to 26200kg/hr, the composition and recovery are follows :

10% decrease in feed flow rate(26200 kg/hr)					
Components	**Top distillate of OMS (Wt fraction)**	**Bottom of OMS (Wt fraction)**		**Top distillate of OMS (Recovery)**	**Bottom of OMS (Recovery)**
Saturate, C_8, C_9	2.27E-02	4.96E-03		9.84E+01	1.57E+00
Toluene	4.83E-03	2.24E-21		1.00E+02	3.38E-18
Ethyl Benzene	0.166368606	5.12E-05		99.99776204	2.24E-03
P – xylene	0.178128396	2.27E-03		99.90750142	9.25E-02
M – xylene	0.452325135	7.69E-03		99.87647228	1.24E-01
O – xylene	0.175658673	4.55E-01		84.15064757	15.84935243
C_9^+ Aromatics	1.23E-05	0.530457688		3.17E-02	99.9682548

If the feed flow rate is decreased by 10%, then the recovery of C_9^+ Aromatics remains same but the recovery of O-Xylene has increased by 2.5%. but decreasing feed flow rate ultimately decrease in production. When we required high recovery of O-Xylene in bottom of OMS, this condition specially recommended.

4.1.4 Table 26.Increased bottom flow rate by 10%:

For 10 % increase in bottom flow rate from 1778 kg/hr to 1956 kg/hr, the composition and recovery are :

10% increase in bottom flow rate(1956 kg/hr)				
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)	Top distillate of OMS(Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.27E-02	4.57E-03	9.86E+01	1.43E+00
Toluene	4.82E-03	2.12E-21	1.00E+02	3.17E-18
Ethyl Benzene	1.66E-01	4.82E-05	99.99791332	2.09E-03
P – xylene	1.78E-01	2.14E-03	99.91370798	8.63E-02
M – xylene	0.452021449	7.25E-03	99.8846907	1.15E-01
O – xylene	0.176199076	4.50E-01	84.47319193	1.55E+01
C_9^+ Aromatics	1.23E-05	5.36E-01	3.20E-02	99.96802145

If the bottom flow rate has increased by 10%, then the recovery of C_9^+ Aromatics remains same but the recovery of O-Xylene has increased by 2.25%. But increasing bottom flow rate ultimately increase the load to the reboiler. When we ENrequired high recovery of O-Xylene in bottom of OMS, this condition also specially recommended.

Table 27.Decreased bottom flow rate by 10%:

For 10 % decrease in bottom flow rate from 1778 kg/hr to 1600kg/hr, the composition and recovery are :

10% decrease in bottom flow rate(1600kg/hr)				
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)	Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.26E-02	1.39E-03	99.64523309	0.354766908
Toluene	4.76E-03	8.28E-22	100	1.01E-18
Ethyl Benzene	0.164103609	1.78E-05	99.99936914	6.31E-04
P – xylene	0.175816859	7.96E-04	99.97368059	2.63E-02
M – xylene	0.446553961	2.71E-03	99.96469443	3.53E-02
O – xylene	0.186103521	0.340350587	90.38631459	9.613685405
C_9^+ Aromatics	1.44E-05	0.654737625	3.77E-02	99.96231232

If the bottom flow rate has decreased by 10%, then the recovery of C_9^+ Aromatics remains unchanged but the recovery of O-Xylene has decreased by 2.75%. But decreasing in bottom flow rate ultimately increase the load to the top trays. This condition may not be used due to less recovery of O-Xylene.

4.1.5 Increased distillate flow rate by 5%:

For 5% increase in distillate flow rate from 27333 kg/hr to 28700 kg/hr, Aspen HYSYS hasn't able converged. It signifies, under this condition the column will

not in safe position or else the product quality will changed. This condition hasn't used at all .

Table 28.Decreased distillate flow rate by 5%:

For 5% decrease in distillate flow rate from 27333 kg/hr to 25966 kg/hr. the composition and recovery are follows :

5% decrease in distillate flow rate(25966kg/hr)				
Components	Top distillate of OMS (Wt fraction)	Bottom of OMS (Wt fraction)	Top distillate of OMS (Recovery)	Bottom of OMS (Recovery)
Saturate, C_8, C_9	2.04E-02	3.07E-02	84.55465307	15.44534693
Toluene	5.05E-03	5.07E-20	100	1.22E-16
Ethyl Benzene	0.173752133	1.22E-03	99.91485107	8.51E-02
P – xylene	0.181916836	3.66E-02	97.61551087	2.384489131
M – xylene	0.459267431	0.116293606	97.01951917	2.980480825
O – xylene	0.159644184	0.482553013	73.16813134	26.83186866
C_9^+ Aromatics	1.01E-05	0.332644156	2.50E-02	99.97499198

If the distillate flow rate has decreased by 5%, then the recovery of C_9^+ Aromatics remains same but the recovery of O-Xylene has increased by 14.25%. But decreasing in distillate flow rate ultimately increase the load to the reboiler. When we required high recovery of O-Xylene in bottom of OMS, this condition specially recommended.

4.1.6 Pressure

This table signifies, the role of pressure on different thermodynamics properties. How the vapour to liquied ratio changes by slightly changing in pressure.

Table 29(Comparision of different Pressure)

	P=2.4 atm	P=2.3 atm	P=2.35 atm	P=2.36 atm
Stream name	1	1	1	1
Vapour	0	1	0.514462826	6.09E-02
Temp °C	175	175	175	175
Pressure(KPa)	243.1799918	233.0474921	238.113742	239.1269919
Molar flow(kg mol/hr)	270.9827832	270.9827832	270.9827832	270.9827832
Mass flow (kg/hr)	29111	29111	29111	29111
Std ideal liquid volume m3/hr	33.73303185	33.73303185	33.73303185	33.73303185
Molar enthalpy(KJ/ kg mole)	-2467.13219	31559.98531	15017.51284	- 400.7831103
Molar entropy KJ/ kg mole C	100.8951119	176.9917078	139.9214141	105.5074704
Heat flow KJ/hr	- 668550.3473	8552212.655	4069487.427	- 108605.3227
Std, liq vol m3/hr	33.59554136	33.59554136	33.59554136	33.59554136
Fluid package	Basis-1	Basis-1	Basis-1	Basis-1

Since our feed is at liquid state, Aspen HYSYS indicate we should go below 2.4 atm. at a particular temperature (175 °C). At 2.3 atm , the feed is total vapor. By increasing 0.05 atm the feed has changed in to partly vapor and partly liquid. So it gives the indication to the operator, if the feed is liquid state we should operate above 2.4 atm. other physical properties has also significantly changed

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4,2 Table 30.Comparision of plant operation data, short-cut, Rigorous calculation:

This table signifies the validation of result between real plant operation, Short-cut and Rigorous calculations. We have seen that Rigorous Calculations has quite similar to real plant operations. Hand calculations by Short-cut method also reasonable good in comparison to real plant operation.

Parameters	Plant operation	Short-cut Method	Rigorous Method
Feed Temp.(^{O}C)	175	175	175
Feed pressure(KPa)	240	230	243
Feed rate(Kg/hr)	29111	29111	29111
Distillate rate(Kg/hr)	27333	27333	27333
Bottom rate(Kg/hr)	1778	1778	1778
Reflux drum Pressure(KPa)	104	-	101.3
Reflux drum Temp(^{O}C)	156	-	139.1
Column top pressure(KPa)	103	101	103.3
Column top temp(^{O}C)	157	145	140.1
Column bottom pressure(KPa)	204	203	202.6
Column bottom temp(^{O}C)	186	183	181.2
Reboiler O/L temp(^{O}C)	187	185	183.1
Reflux ratio	2.5	3.5	2.5
Condenser Duty (KJ/hr)	3.42 e+007	-	3.26796 e+007
Reboiler Duty (KJ/hr)	3.11 e+007	-	3.056 e+007
Overhead Product rate(Kg/hr)	27333	27333	27333
Number of trays	126	127	126

CONCLUSION AND RECOMMENDATION

In the present work, a mathematical model has been developed for multi-stage, multi-component, simple distillation column. Modeling and simulation has done by Aspen HYSYS 2004 version. It has given flexibility in product quality, duties, temperature, pressure, liquid to vapor ratio, etc. We have undergone the detailed sensitivity analysis, which signified the product qualities of different operating conditions.

We also did the hand calculation by shortcut method. Comparing the real plant operation data with shortcut and rigorous calculations. For large number of components but a fewer number of plates modified Tomich method is suggested and for problem having large number of plates with fewer number of component Naphtali-Sandholm procedure generally used.

Since Ortho-meta splitter has fewer number of components and large number of plates, hence Naphtali-Sandholm method is recommended.

The equations involved in mathematical model are non-linear algebraic equation and can be solved by numerical methods using mathematics software like Matlab, Mathematica etc. Newton-Raphson and Thomas algorithm are the best numerical methods for solving these types of equations. The results obtain from numerical solutions can be used for on line optimization.

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