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DESIGN DISTILLATION COLUMN FOR SEPARATION OF ORTHO , META , PARA NITRO TOLUENE AND OPTIMIZATION USING ASPEN HYSYS 3.2

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ABSTRACT

Aspen Hysys 3.2 is simulation software used for simulation of chemical process .It is market leading process modeling tool for conceptual design , optimization ,asset management & performance monitoring .Distillation is one the most common industrial separation process .Efforts have been made by researchers to various design method , minimize energy consumption ,optimization and capital cost by inventing analytical and graphical design method . This paper shows the case study for design multi component distillation column Ortho Nitro Toluene , Meta Nitro Toluene & Para Nitro Toluene by analytical method as well Aspen hysys 3.2.

Keywords : Aspen HYSYS, Multi component Distillation, Isomer Separation, Packed column, simulation of distillation column.

I.INTRODUCTION

Table 1: Preliminary calculation Data

	ONT	**MNT**	**PNT**
Molecular Weight	137.13	137.13	137.13
Boiling point °C	221.7	232.6	238.3
Specific Gravity	1.162	1.286	1.157

Design of the Distillation column

We have mixture of Ortho , Meta , Para Nitro Toluene which has to be separated at purity of MNT more than 95 % , ONT & PNT should be more than 99 % .Flow rate of the feed is 25000 kg/hr which contains mole fraction of ONT = 60% (15000 Kg/hr), MNT = 6% (1500Kg/hr) , PNT = 34% (8500 Kg/hr)

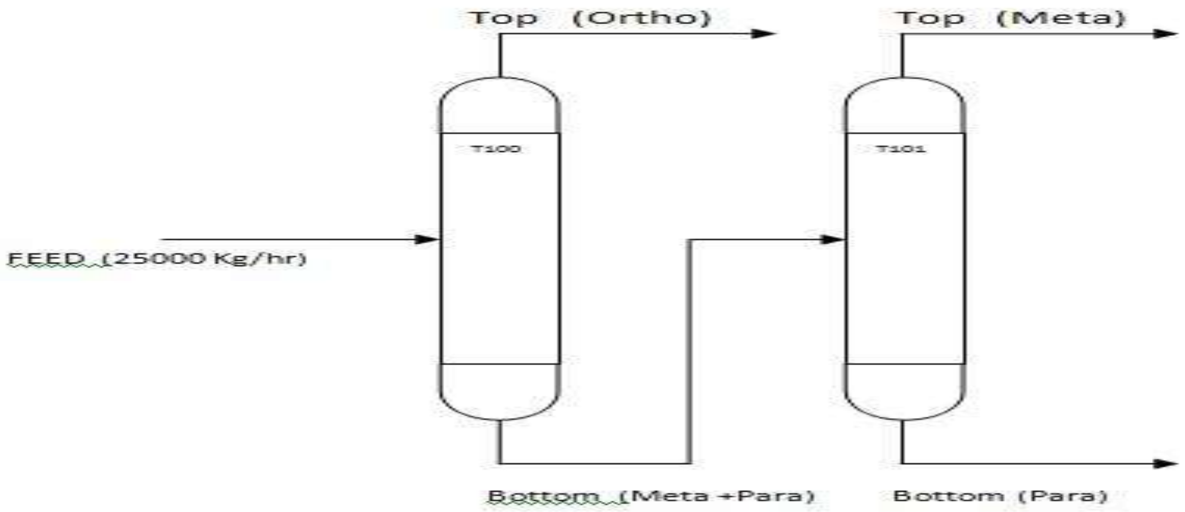

Table 2 Calculation of vapor pressure using Antoine constant at 140 ^{0} C

	ONT	MNT	PNT
T ^{0} C	140.3	140.3	140.3
$\frac{B}{T+C}$	5.853426	6.112369	6.437824
$\frac{A-B}{T+C}$	1.837944	1.752971	1.664856
mmHg(Abs)	68.86	56.62	46.22

Table 3 Relative volatility of component of feed to column No-T 101

Relative Volatility (O/M)	$\frac{68.85}{56.62}$= 1. 21
Relative Volatility (M/P)	$\frac{56.62}{46.22}$= 1. 22
Relative Volatility (O/P)	$\frac{68.85}{46.22}$ = 1. 48

Geometric Average of relative volatility (used for FENKES's equation)

=1.30

Bubble point was calculated as follows

$Y_a = \frac{Xa\ Pa°}{TP}$

Where ,

Y_a= Vapor pressure , X_a= Mole Fraction , $Pa°$ =Partial Pressure of individual component

T_p = Total pressure

Table 4: Bubble point calculation

		Feed mole fraction	**Re boiler pressure (abs mmHg)**
ONT	0.68856	0.6	60
MNT	0.05662	0.06	60
PNT	0.261929	0.34	60

Corresponding bubble point with 60 mmHg pressure at 140 °C Mole fraction was calculated.

Table 5 : Mole fraction of the distillate and bottom of column No- T 101

	ONT	**MNT**	**PNT**	**Total**
Distillate mole fractions	0.995	0.005	0	1
Bottom mole fraction	0.005	0.1429	0.8621	1

Now we select light key and heavy component

Table 6 : Heavy and light keys component in distillate and bottom of T 101

Light key in distillate	O N T
Heavy key in distillate	M N T
Heavy key in Bottom	P N T
Light key in Bottom	M N T

Calculation of minimum no of stages

Ratio of light key to heavy key component in distillate , $\frac{0.995}{0.005} = 199$

Ratio of heavy to light key component in bottom , $\frac{0.8521}{0.1429} = 5.96$

Minimum no of stages can be calculated as

$$=\left(\frac{\log(5.96\times199)}{\log mean\ (Relative\ volatility\ of\ at\ bubble\ temperature\ )}\right) = \frac{7.07}{0.3}$$

= Minimum No of stages are 26.94 =27

FUG Method does not give information about feed tray location .feed tray location can be determine by using following equation (Kirkbride Equation)

$$\text{Log}\left\{\frac{Nr}{Ns}\right\} = \left[0.206 \log \left(\frac{B}{D}\right)\left(\frac{X,HK}{X,LK}\right)_f \left(\frac{Xb\ ,LK}{Xd\ ,HK}\right)^2\right]$$

N_r = 12 N_s = 15

Using ***Underwood's*** second equation (at q≈1):

$$1-q=\sum\frac{\alpha_i x_{if}}{\alpha_i-\theta} \qquad (1)$$

Now here onwards we need to solve Underwood equation which will give value of 0.88 or nearby, For that we need to solve Underwood equation assuming θ = 2.82

E.g. for O N T =$(\frac{1.22\times 0.6}{1.2-2.8})$ = -0.4549

Table 7 Value of X_f for Underwood equation

ONT	**MNT**	**PNT**	**Total**
0.45	-0.45	-0.37	-0.04

$$\left(\frac{L}{D}\right)_{\min} = \left(\frac{1-\{(\sum \text{O,P,M (Mole fraction in distillate}\times\alpha)\}}{(\alpha-\theta)}\right)$$

After getting value of θ now we have to calculate value for $(\frac{L}{D})_{\min}$

Table 8: Calculation of $(\frac{L}{D})_{min}$ for each component.

ONT	**MNT**	**PNT**	**Total**
-0.75	0.003	0.0000270	-0.75

$$\left(\frac{L}{D}\right)_{\min} = \left(\frac{1-\{(\sum \text{O,P,M (Mole fraction in distillate}\times\alpha)\}}{(\alpha-\theta)}\right)$$

=1-(-0.75) =1.75

Now calculating optimum reflux ratio

=1.2 ×1.75

Optimum Reflux ration=2.10

Design of 2nd column T 102

Table 9 Calculation of vapor pressure using Antoine constant at 150 C ^{0}

	ONT	**MNT**	**PNT**
T (C ^{0})	150.353	150.353	150.353
$\frac{B}{T+C}$	5.702224	5.964183	6.2879

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$\frac{A-B}{T+C}$	1.989146	1.901157	1.8147
mmHg	97.53182	79.64466	65.2753

Table 10 Relative volatility of component of feed to column No-T 102

Relative Volatility (O/M)	1.224587006
Relative Volatility (M/P)	1.220134666
Relative Volatility (O/P)	1.494161057

Geometric Average of relative volatility (used for FENKES's equation)

=1.30

Bubble point was calculated as follows

$$Y_a = \frac{Xa\ Pa°}{TP}$$

Where ,

Y_a= Vapor pressure , X_a= Mole Fraction , $Pa°$ =Partial Pressure of individual component

T_p = Total pressure

Table 11 : Mole fraction of feed to column No- T 102

		Feed mole fraction	**Re boiler pressure (abs mmHg)**
ONT	0.007225	0.005	67.5
MNT	0.168611	0.1429	67.5
PNT	0.824016	0.8521	67.5

Table 12 : Mole fraction of the distillate and bottom of column No- T 102

	ONT	**MNT**	**PNT**	**Total**
Distillate mole fractions	0.033	0.940	0.027	1
Bottom mole fraction	0.000	0.00056	0.99943	1

Now we select light key and heavy component

Table 13: Heavy and light keys component in distillate and bottom of T 102

Light key in distillate	M N T
Heavy key in distillate	P N T
Heavy key in Bottom	P N T
Light key in Bottom	M N T

Calculation of minimum no of stages

Ratio of light key to heavy key component in distillate , $\frac{0.94}{0.027} = 34.81$

Ratio of heavy to light key component in bottom , $\frac{0.9994}{0.00056}$=1784.64

Minimum no of stages can be calculated as

$$=\left(\frac{\log(34\times1784.64)}{\log mean \ (Relative \ volatility \ of \ at \ bubble \ temperature \ )}\right)$$

= Minimum No of stages are 41.24 =42

FUG Method does not give information about feed tray location .feed tray location can be determine by using following equation (Kirkbride Equation)

$$\text{Log}\left\{\frac{Nr}{Ns}\right\} = \left[0.206 \log \left(\frac{B}{D}\right)\left(\frac{X,HK}{X,LK}\right)_f \left(\frac{Xb\ ,LK}{Xd\ ,HK}\right)^2\right]$$

N_r = 7 N_s = 35

Using ***Underwood*'s** second equation (at q≈1):

$$1 - q = \sum\frac{\alpha_i x_{if}}{\alpha_i - \theta} \qquad (1)$$

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Now here onwards we need to solve Underwood equation which will give value of 0.88 or nearby,

For that we need to solve Underwood equation assuming θ = 2.51

E.g. for O N T =$\left(\frac{1.22\times 0.005}{1.22-2.51}\right)$ = -0.0047

Table 14 Value of X_f for Underwood equation

ONT	MNT	PNT	Total
-0.004754357	-0.13	-1.25	-1.38

$$\left(\frac{L}{D}\right)_{min} = \left(\frac{1-\{(\sum O,P,M\ (\text{Mole fraction in distillate}\times\alpha)\}}{(\alpha-\theta)}\right)$$

After getting value of θ now we have to calculate value for $\left(\frac{L}{D}\right)_{min}$

Table 15: Calculation of $\left(\frac{L}{D}\right)_{min}$ for each component.

ONT	MNT	PNT	Total
-0.0323	-0.907	-0.0073	-0.946

$$\left(\frac{L}{D}\right)_{min} = \left(\frac{1-\{(\sum O,P,M\ (\text{Mole fraction in distillate}\times\alpha)\}}{(\alpha-\theta)}\right)$$

=1-(-0.946) =1.946

Now calculating optimum reflux ratio

=1.2 ×1.946

=2.33

R+1= 3.33

Optimum reflux ration =3.33

Now same column we will simulate using Aspen Hysys

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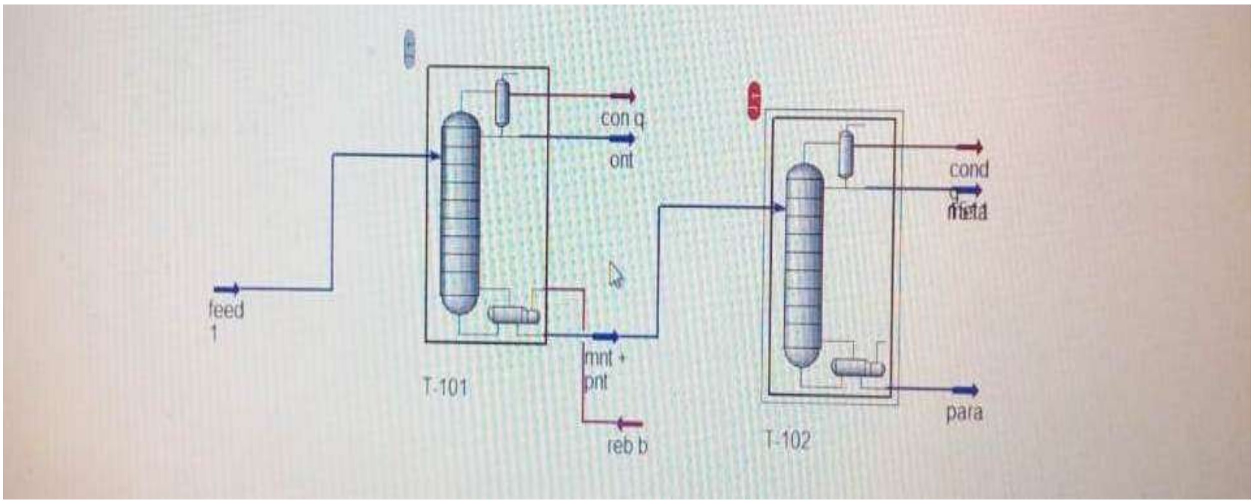

Figure 2: Column pictorial

Note -NRTL model is used to simulate column

Table 16: Showing column performance through HYSYS

Column Parameter	Result
Minimum no of trays	40
Actual no of trays	80
Optimal feed stages	28.7
Condenser Temperature (°C)	136
Re boiler Temperature (°C)	150

Table 17: Shows Distillate & Bottom of column No- T 101.

	Flow rate Kg/Hr	ONT Wt %	MNT Wt %	PNT Wt %
Feed	9974	0.50	14.29	85.21
Distillate	1511.2121	3.3	94.00	2.7
Bottom	8462.7879	0.00	0.056	99.94

Table 18: Shows Distillate & Bottom of column No- T 102.

Component Name	Mass Fraction in Distillate	Flow rate (Kg/Hr)	Mass Fraction in Bottom	Flow rate (Kg/Hr)
ONT	0.3	43.17	0	0
MNT	0.01	1381.44	0.005	42.675
PNT	0.96	7.195	0.995	8492.33

Optimization of Feed point location through HYSYS of column T 101

Three different location of feed point were chosen for the feed location optimization

Table 19: Shows comparison various feed point location of column No- T 101

	Feed stage	**10**	**29**	**65**
Top of T101	Temperature(^{o} C)	137.1	136.8	137.7
	Pressure (Kpa)	8.00	8.00	8.00
	Mass Fract. ONT	0.92	0.9634	0.9783
	Mass Fract.MNT	0.0262	0.0197	0.0217
	Mass Fract. PNT	0.0480	0.0169	0.000
	Mass flow (Kg/Hr)	14950	15000	15020

Bottom of T101	Temperature(^{O} C)	148.9	149.7	150.
	Pressure(Kpa)	9.00	9.00	9.00
	Mass Fract ONT	0.1150	0.0550	0.0308
	Mass Fract.MNT	0.1103	0.1204	0.1179
	Mass Fract. PNT	0.7747	0.8246	0.8517
	Mass flow (Kg/Hr)	10050	10000	9981
Rectification Stages		10	29	65
Stripping stages		69	50	14

If we see above 3 results it shows that as we goes to increase the stages in rectification section get more purity of ONT in distillate.

Optimization of Feed point location through HYSYS of Column T102

Three different location of feed point were chosen for the feed location optimization

Table 20: Shows comparison various feed point location of column No- T 102

	Feed stage	40	72	95
Top of T102	Temperature(^{O} C)	142.1	142.0	142.0
	Pressure (Kpa)	8.00	8.00	8.00

	Mass Fract. ONT	0.0390	0.0390	0.0387
	Mass Fract.MNT	0.9570	0.9610	0.9238
	Mass Fract. PNT	0.0040	0.0000	0.0375
	Mass flow (Kg/Hr)	1450	1440	1490
Bottom of T102	Temperature(^{o} C)	151	151	151
	Pressure(Kpa)	9	9	9
	Mass Fract ONT	0	0	0
	Mass Fract.MNT	0.0114	0.0118	0.0128
	Mass Fract. PNT	0.9969	0.9964	0.9872
	Mass flow (Kg/Hr)	8525	8535	8485
Rectification Stages		40	72	95
Stripping stages		68	36	13

Mass balance across column T 101

Table 2 Showing mass balance at Column No T-101

	ONT	MNT	PNT	Total
Feed to T 101	15000	1500	8500	25000
Distillate of T 101	14699.93	318.100	0	15018
Bottom of T 101	49.87	1424.85	8499.28	9974

(all value are in Kg/hr)

Mass balance across column T 102

Table 3 Showing mass balance at Column No T-102

	ONT	MNT	PNT	Total
Feed to T 102	49.87	1424.85	8499.28	9974
Distillate of T 102	49.87	1382	0	1431.87
Bottom of T 102	0	42.84	8499.28	8542.13

(all value are in Kg/hr)

Column diameter was calculated for both the column.

Table 20 Diameter for column No T-101 & T- 102

	Rectifying Section	Stripping Section
Column No T-101	2.84	2.79
Column No T-102	1.80	1.76

Tray spacing was 0.5 m

II.RESULT

	Column T101		Column T102	
	By calculation	By Aspen Hysys	By Calculation	By Aspen Hysys
Minimum number of stages required	27	40	42	57
Top temperature ^{O} C	120	136.6	125	142

Bottom temperature ^{o} C	140	150.3	150.35	151.2
Column top pressure(mmHg)abs	32	64	35	60.02
Column bottom pressure(mmHg)abs	60	120	67.5	67.52

III.CONCLUSION

Initially manual calculation was done for the column which took lot of time, but later optimization was done on HYSYS software which gave instant and good results proving to point that designing through HYSYS gives saves lot of time. Through HYSYS we manage to get Ortho and Para fraction at purity of 99.50 % while Meta was obtained at purity of 96.55 % . Both column was operated under vacuum. And decided use same column model with addition of one more batch distillation column for further purification of Top material of column T102.

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