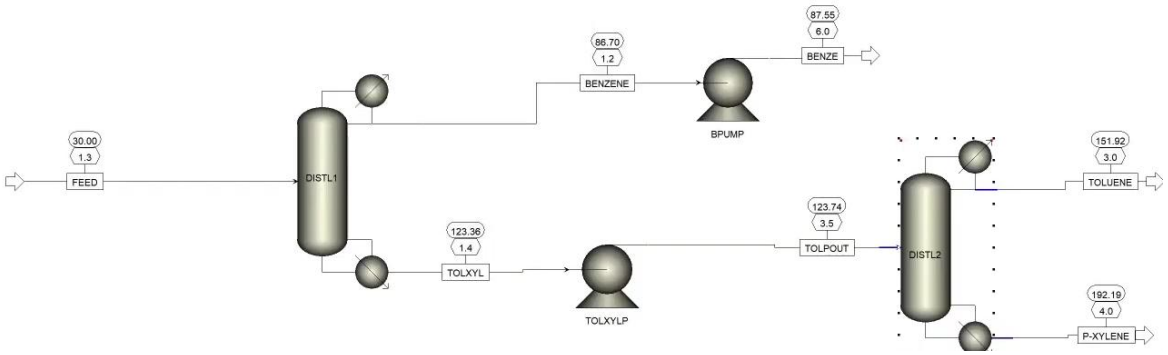
PFD



Abstract

This project focuses on the separation of a ternary BTX mixture—benzene (400 kg/h), toluene (600 kg/h), and p-xylene (100 kg/h)—at 30 °C and 1.3 bar using both shortcut and rigorous distillation methods in Aspen Plus. The separation target is to obtain benzene and toluene with purities of at least 95%, with final product pressures of 6 bar (benzene), 3 bar (toluene), and 4 bar (p-xylene).

The workflow begins with verification of component boiling points and vapour–liquid equilibrium through Flash calculations. K-value analysis confirms the volatility order benzene > toluene > p-xylene, enabling correct identification of light and heavy keys. The average relative volatility for the first column (benzene/toluene) is approximately 2.19.

Shortcut column design is performed using the Fenske–Underwood–Gilliland method. Fenske's equation gives a minimum of about 6.92 theoretical stages. Underwood's method determines the minimum reflux ratio, while Gilliland's correlation relates operating reflux to actual stage count. These estimates are implemented using Aspen Plus's DSTWU block, which predicts a benzene purity of roughly 96.13% in the distillate.

A rigorous column model (Distl/RADFRAC) is then developed using stagewise mass and energy balances, tray efficiencies, and condenser/reboiler specifications. The rigorous simulation yields a practical benzene purity of approximately 95.2%, which is expected to be slightly lower than DSTWU due to real-stage inefficiencies and non-ideal VLE behavior.

The second column (toluene/p-xylene) includes the effects of benzene carryover, requiring iterative optimization of reflux and feed stage location. Final purities and recoveries are validated using rigorous simulation.

This combination of shortcut estimation and detailed modelling provides an efficient and accurate design approach for BTX separation, highlighting best practices for multicomponent distillation workflows.

BTX Separation through distillation column

Steps -1

Boiling point calculation of every component

Benzene	Toluene		
88.44	119.64	147.94	

Step-2

Phase equilibrium data of every component with k|

Benzene

Component	F	X	Y	K
BENZENE	0.407234	0.407234	0.64689	1.00707
TOLUENE	0.517859	0.517859	0.33396	0.408843
P-XYLENE	0.0749066	0.0749066	0.01915	0.162078

Toluene

Component	F	X	Y	K
BENZENE	0.407234	0.215777	0.407234	2.16368
TOLUENE	0.517859	0.595158	0.517859	0.997547
P-XYLENE	0.0749066	0.189065	0.0749066	0.454215

p-xylene

Component	F	X	Y	K
BENZENE	0.407234	0.237371	0.407234	3.79945
TOLUENE	0.517859	0.590749	0.517859	1.94139
P-XYLENE	0.0749066	0.171881	0.0749066	0.965154

K benzene>K toluene>K xylene

so Benzene is light key and toluene is heavy key then calculate relative volatility is ratio of light key to the heavy key

step-3

Average rekative volatility =2.19

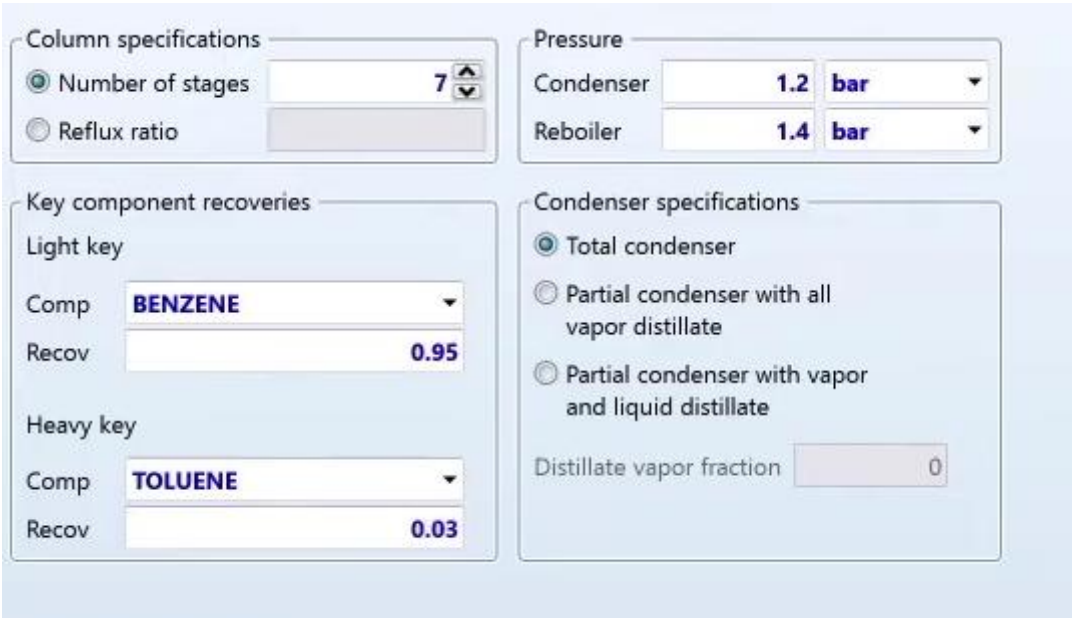
1.00707	2.16368	3.79945			
0.408843	0.997547	1.94139			
2.46321938	2.16900056	1.95707715	2.19643236		
			2.18670518	rel vol	2.19

Step-4 (calculate minium number of trays by the help of Fenske method)

1.00707	2.16368	3.79945			
0.408843	0.997547	1.94139			
2.46321938	2.16900056	1.95707715	2.19643236		
			2.18670518	rel vol	2.19
				xD	0.95
				XB	0.075
				Nm	6.9610076

Nm=6.916

Step-5 (use DSTWU method to calculate mole fraction)



Minimum reflux ratio	1.0722	
Actual reflux ratio	59.1903	
Minimum number of stages	6.81295	
Number of actual stages	7	
Feed stage	4.10339	
Number of actual stages above feec	3.10339	
Reboiler heating required	678845	cal/sec
Condenser cooling required	667453	cal/sec
Distillate temperature	87.6394	C
Bottom temperature	123.698	C
Distillate to feed fraction	0.425732	
HETP		

Reflux ratio is not fit

So do again and change in recovery of heavy key

Minimum reflux ratio	1.34832	
Actual reflux ratio	1.68601	
Minimum number of stages	7.93976	
Number of actual stages	15.8795	
Feed stage	9.16468	
Number of actual stages above feec	8.16468	
Reboiler heating required	39157.9	cal/sec
Condenser cooling required	27716.2	cal/sec
Distillate temperature	86.5191	C
Bottom temperature	123.648	C
Distillate to feed fraction	0.402411	
HETP		

now everything is good

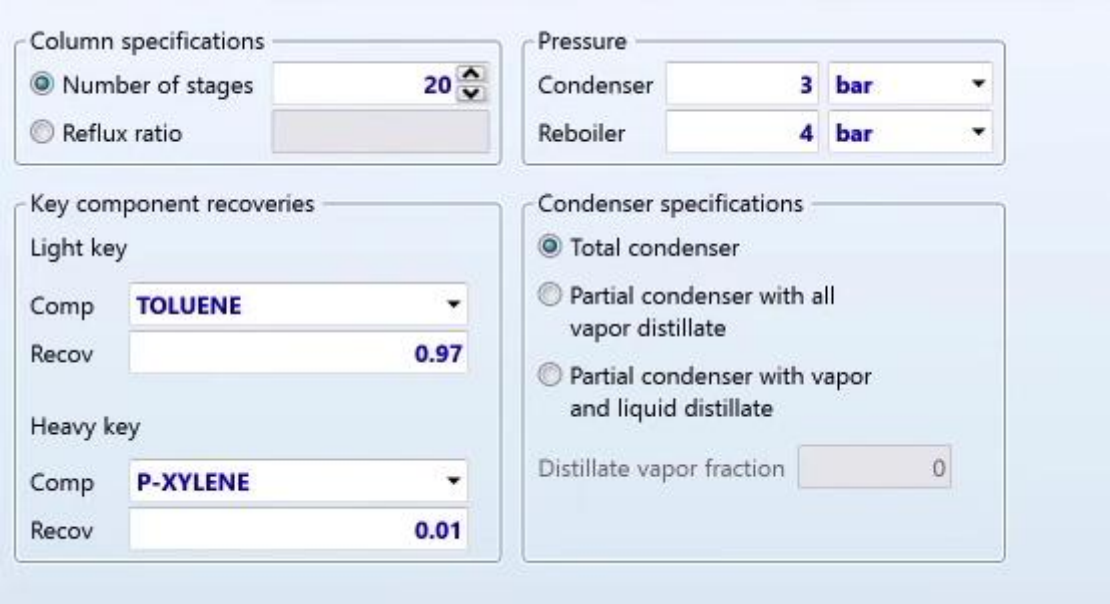
	Units	FEED	BENZENE	TOLXYL	
− MIXED Substream					
Phase		Liquid Phase	Liquid Phase	Liquid Phase	
Temperature	C	30	86.5191	123.648	
Pressure	bar	1.3	1.2	1.4	
Molar Vapor Fraction		0	0	0	
Molar Liquid Fraction		1	1	1	
Molar Solid Fraction		0	0	0	
Mass Vapor Fraction		0	0	0	
Mass Liquid Fraction		1	1	1	
Mass Solid Fraction		0	0	0	
Molar Enthalpy	cal/mol	5937.56	13520.5	6312.82	
Mass Enthalpy	cal/gm	67.8741	171.895	67.5741	
Molar Entropy	cal/mol-K	-72.8285	-54.395	-71.0939	
Mass Entropy	cal/gm-K	-0.832525	-0.691561	-0.761008	
Molar Density	mol/cc	0.00982809	0.0102604	0.00820121	
Mass Density	gm/cc	0.859751	0.807034	0.766163	
Enthalpy Flow	cal/sec	20739.3	19004.2	13176.9	
Average MW		87.479	78.6554	93.4208	
+ Mole Flows	**kmol/hr**	**12.5744**	**5.0601**	**7.51435**	
− Mole Fractions					
BENZENE		0.407234	0.961386	0.0340731	
TOLUENE		0.517859	0.0386067	0.940584	
P-XYLENE		0.0749066	7.18144e-06	0.125343	
+ Mass Flows	**kg/hr**	**1100**	**398.004**	**701.996**	

Here Benzene is 96.13%

now use dist model for correct calculation

	Units	FEED	BENZENE	TOLXYL	
Temperature	C	30	86.6957	123.358	
Pressure	bar	1.3	1.2	1.4	
Molar Vapor Fraction		0	0	0	
Molar Liquid Fraction		1	1	1	
Molar Solid Fraction		0	0	0	
Mass Vapor Fraction		0	0	0	
Mass Liquid Fraction		1	1	1	
Mass Solid Fraction		0	0	0	
Molar Enthalpy	cal/mol	5937.56	13457.7	6354.44	
Mass Enthalpy	cal/gm	67.8741	170.84	68.0849	
Molar Entropy	cal/mol-K	-72.8285	-54.4898	-70.957	
Mass Entropy	cal/gm-K	-0.832525	-0.691727	-0.760271	
Molar Density	mol/cc	0.00982809	0.0102416	0.0082119	
Mass Density	gm/cc	0.859751	0.806771	0.766426	
Enthalpy Flow	cal/sec	20739.3	18896.6	13272.9	
Average MW		87.479	78.7736	93.3311	
+ Mole Flows	**kmol/hr**	**12.5744**	**5.05493**	**7.51952**	
− Mole Fractions					
BENZENE		0.407234	0.952958	0.0403767	
TOLUENE		0.517859	0.0470366	0.834365	
P-XYLENE		0.0749066	5.76001e-06	0.125258	
+ Mass Flows	**kg/hr**	**1100**	**398.195**	**701.805**	
+ Mass Fractions					
Volume Flow	l/min	21.324	8.2261	15.2614	

In distil model finally we recived 95.2% benzene
now we move for sepration of toluene and xylene with DSTWU model



Here everthing good now check recovery of toluene

▶	Minimum reflux ratio	1.28069	
	Actual reflux ratio	1.46318	
	Minimum number of stages	12.8837	
	Number of actual stages	30	
	Feed stage	16.9363	
	Number of actual stages above feec	15.9363	
	Reboiler heating required	35494.7	cal/sec
	Condenser cooling required	31921.6	cal/sec
	Distillate temperature	151.926	C
	Bottom temperature	192.336	C
	Distillate to feed fraction	0.850963	
	HETP		

	Units	TOLPOUT	P-XYLENE	TOLUENE	
Mass Vapor Fraction		0	0	0	
Mass Liquid Fraction		1	1	1	
Mass Solid Fraction		0	0	0	
Molar Enthalpy	cal/mol	6375.1	4085.51	8786.34	
Mass Enthalpy	cal/gm	68.3062	39.3551	96.0302	
Molar Entropy	cal/mol-K	-70.9206	-80.5127	-65.1661	
Mass Entropy	cal/gm-K	-0.759881	-0.775567	-0.712231	
Molar Density	mol/cc	0.0082075	0.00666744	0.00802707	
Mass Density	gm/cc	0.766016	0.692157	0.734442	
Enthalpy Flow	cal/sec	13316	1271.83	15617.3	
Average MW		93.3311	103.811	91.4956	
− Mole Flows	**kmol/hr**	**7.51952**	**1.12069**	**6.39883**	
BENZENE	kmol/hr	0.303613	5.26186e-06	0.303608	
TOLUENE	kmol/hr	6.27403	0.188221	6.08581	
P-XYLENE	kmol/hr	0.94188	0.932461	0.0094188	
− Mole Fractions					
BENZENE		0.0403767	4.69521e-06	0.0474474	
TOLUENE		0.834365	0.167951	0.951081	
P-XYLENE		0.125258	0.832044	0.00147196	
+ Mass Flows	**kg/hr**	**701.805**	**116.34**	**585.465**	
+ Mass Fractions					
Volume Flow	l/min	15.2696	2.80139	13.2859	
+ Liquid Phase					

Toulene =95.1%

Do with Distl Model

Simulate in distl model

Toluene recovery

	Units	TOLPOUT	P-XYLENE	TOLUENE	
Phase		Liquid Phase	Liquid Phase	Liquid Phase	
Temperature	C	123.738	192.187	151.919	
Pressure	bar	3.5	4	3	
Molar Vapor Fraction		0	0	0	
Molar Liquid Fraction		1	1	1	
Molar Solid Fraction		0	0	0	
Mass Vapor Fraction		0	0	0	
Mass Liquid Fraction		1	1	1	
Mass Solid Fraction		0	0	0	
Molar Enthalpy	cal/mol	6375.1	4108.76	8788.05	
Mass Enthalpy	cal/gm	68.3062	39.6016	96.0525	
Molar Entropy	cal/mol-K	-70.9206	-80.4197	-65.1632	
Mass Entropy	cal/gm-K	-0.759881	-0.775112	-0.712228	
Molar Density	mol/cc	0.0082075	0.00667252	0.00802746	
Mass Density	gm/cc	0.766016	0.69229	0.734449	
Enthalpy Flow	cal/sec	13316	1287.33	15602.7	
Average MW		93.3311	103.752	91.4921	
+ Mole Flows	**kmol/hr**	**7.51952**	**1.12793**	**6.39159**	
− Mole Fractions					
BENZENE		0.0403767	3.4907e-06	0.0475013	
TOLUENE		0.834365	0.172167	0.951224	
P-XYLENE		0.125258	0.82783	0.00127468	
+ Mass Flows	**kg/hr**	**701.805**	**117.025**	**584.78**	
+ Mass Fractions					

not matched with given result because of bezene is also in feed of second distillation