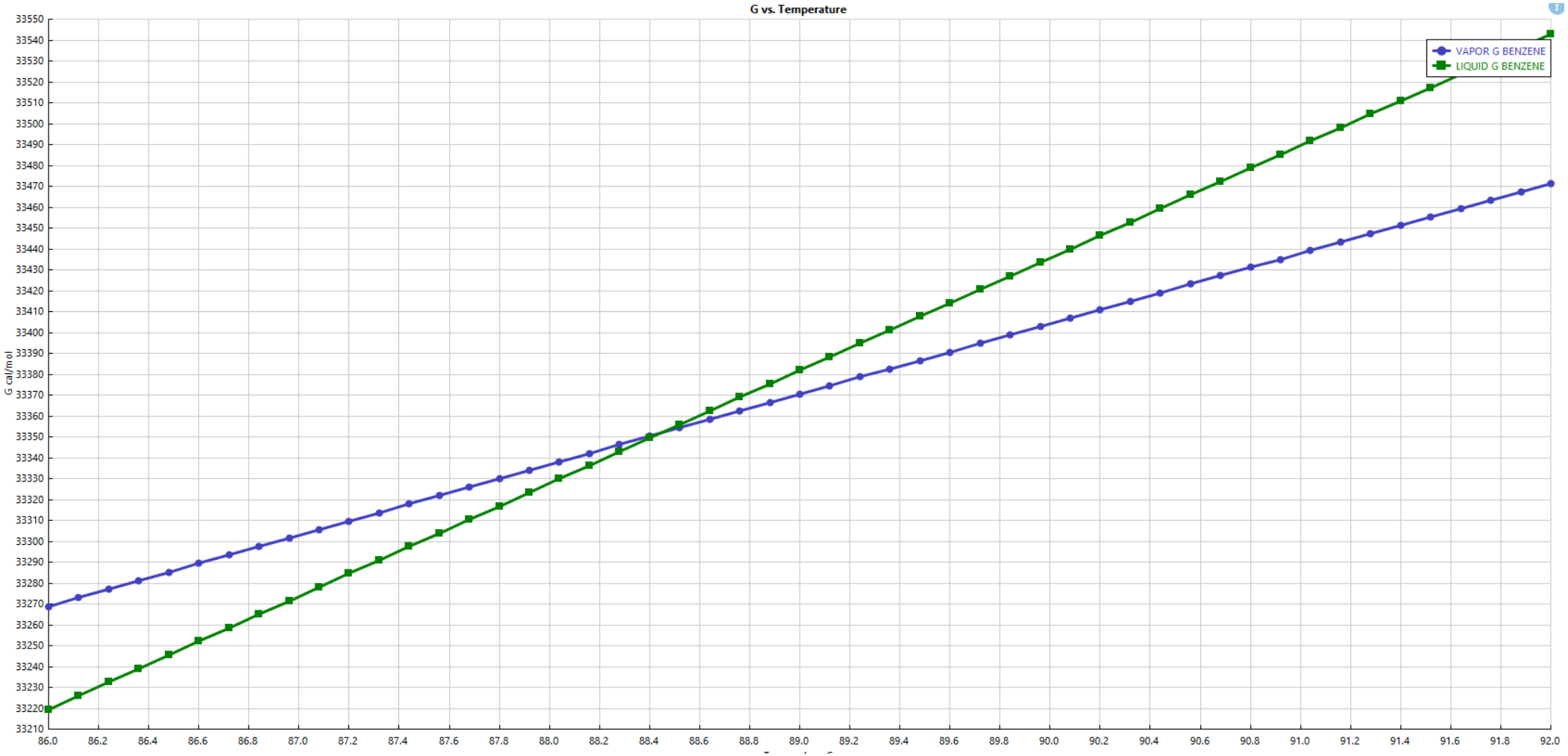
Case Study:

A mixture of benzene (400 kg/h), toluene (600 kg/h) and p-xylene (100 kg/h) at 30 °C and 1.3 bar needs to be separated via distillation with minimum purity of 95% benzene, and 97% toluene. The downstream pressures of benzene, toluene, and p-xylene lines should be 6, 3 and 4 bars respectively. Following strategies should be adopted:

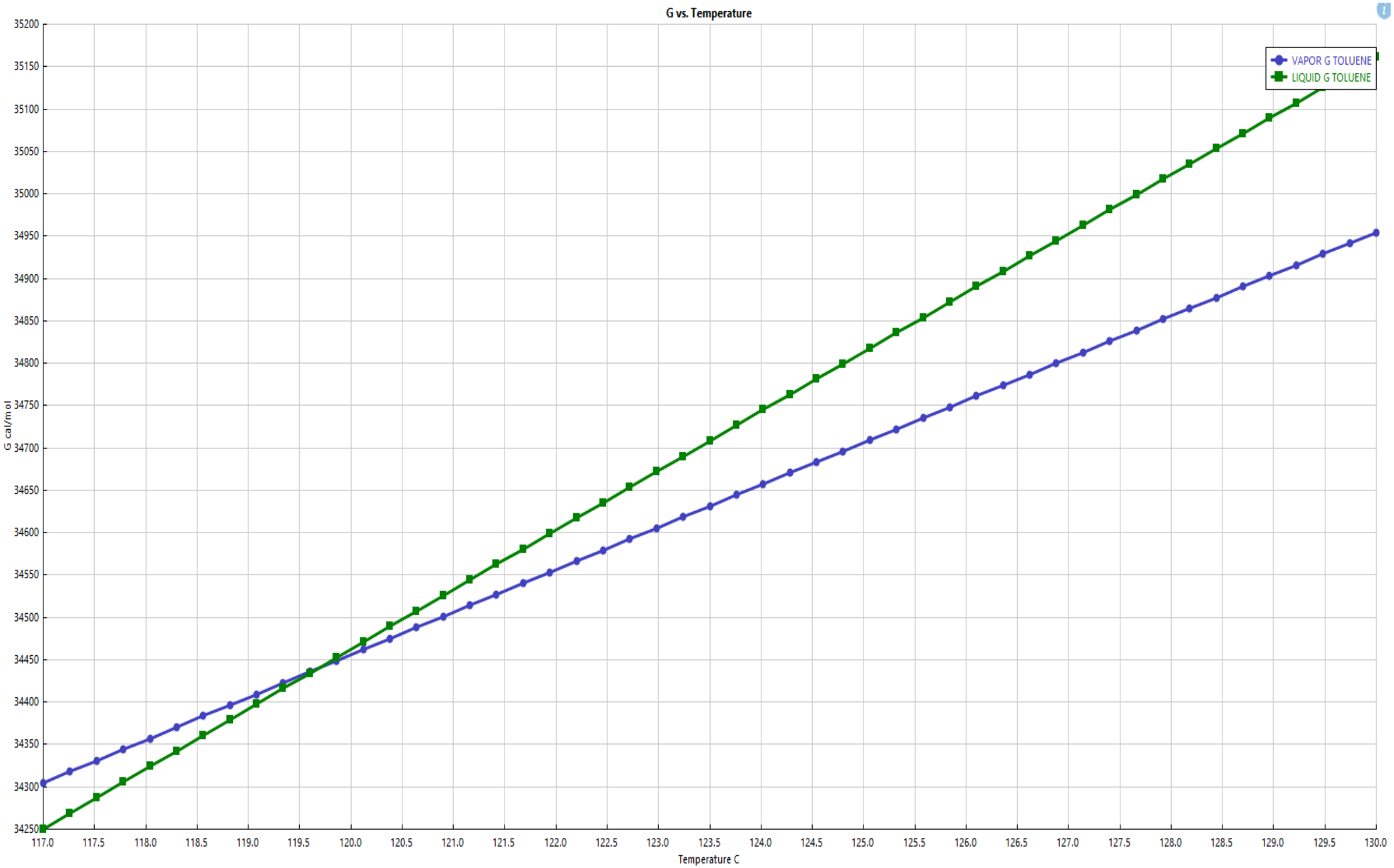
- Verification of boiling points of each component using physical property methods, viz. Pure Component and PT envelope
- Verification of K values and relative volatilities of each component (light and heavy keys) using “Flash” block simulation
- Find minimum reflux ratio and/or minimum number of stages using DSTWU model. Optimize RR vs. stages.
- Simulate real condition using “Dist1” block
- Verify purity of all distilled components and their exit condition after the overall simulation

Pure Component Ananlysis:

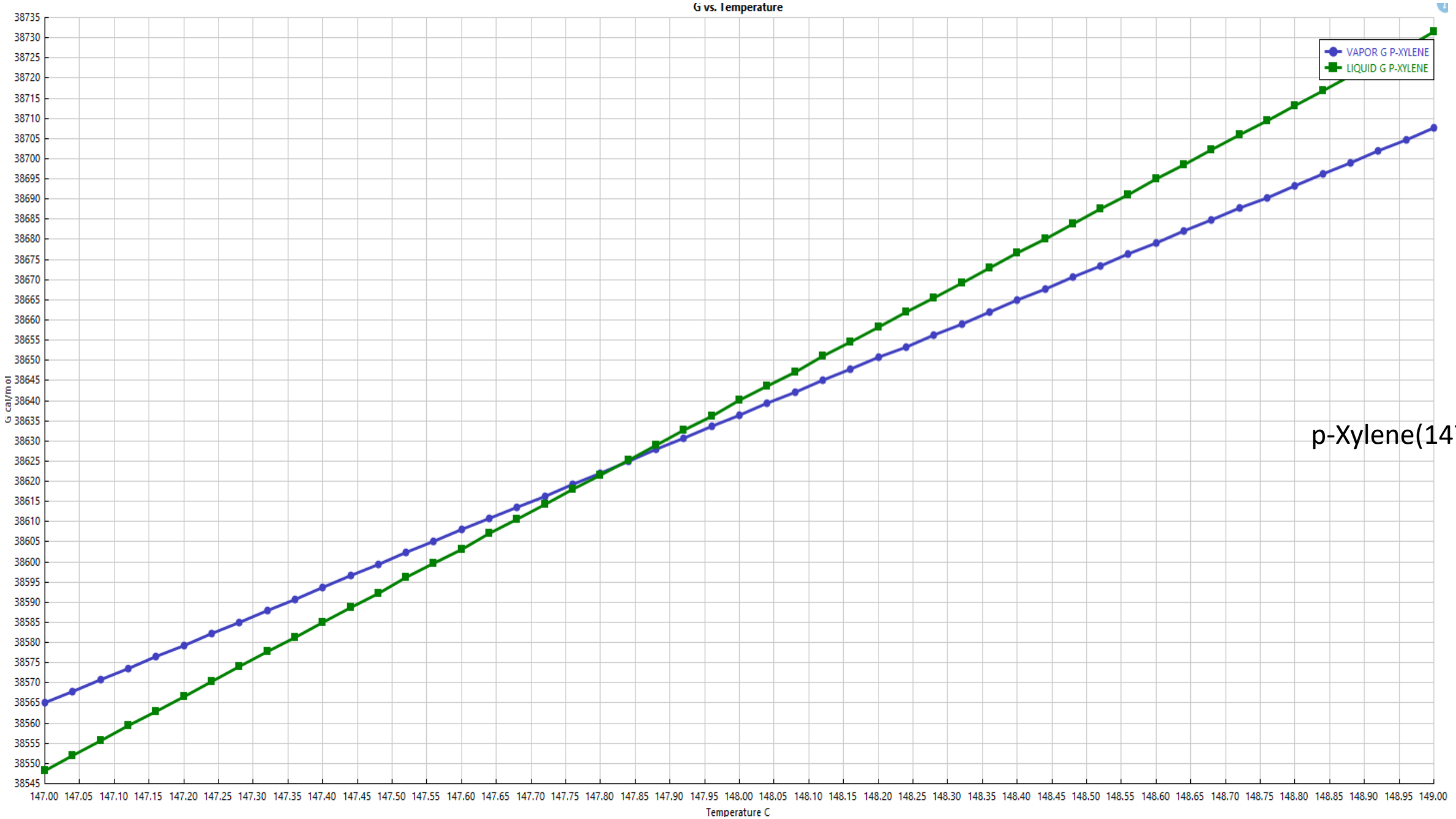
Individual Boiling Point of all three components at 1.3 bar



Benzene (88.44°C)

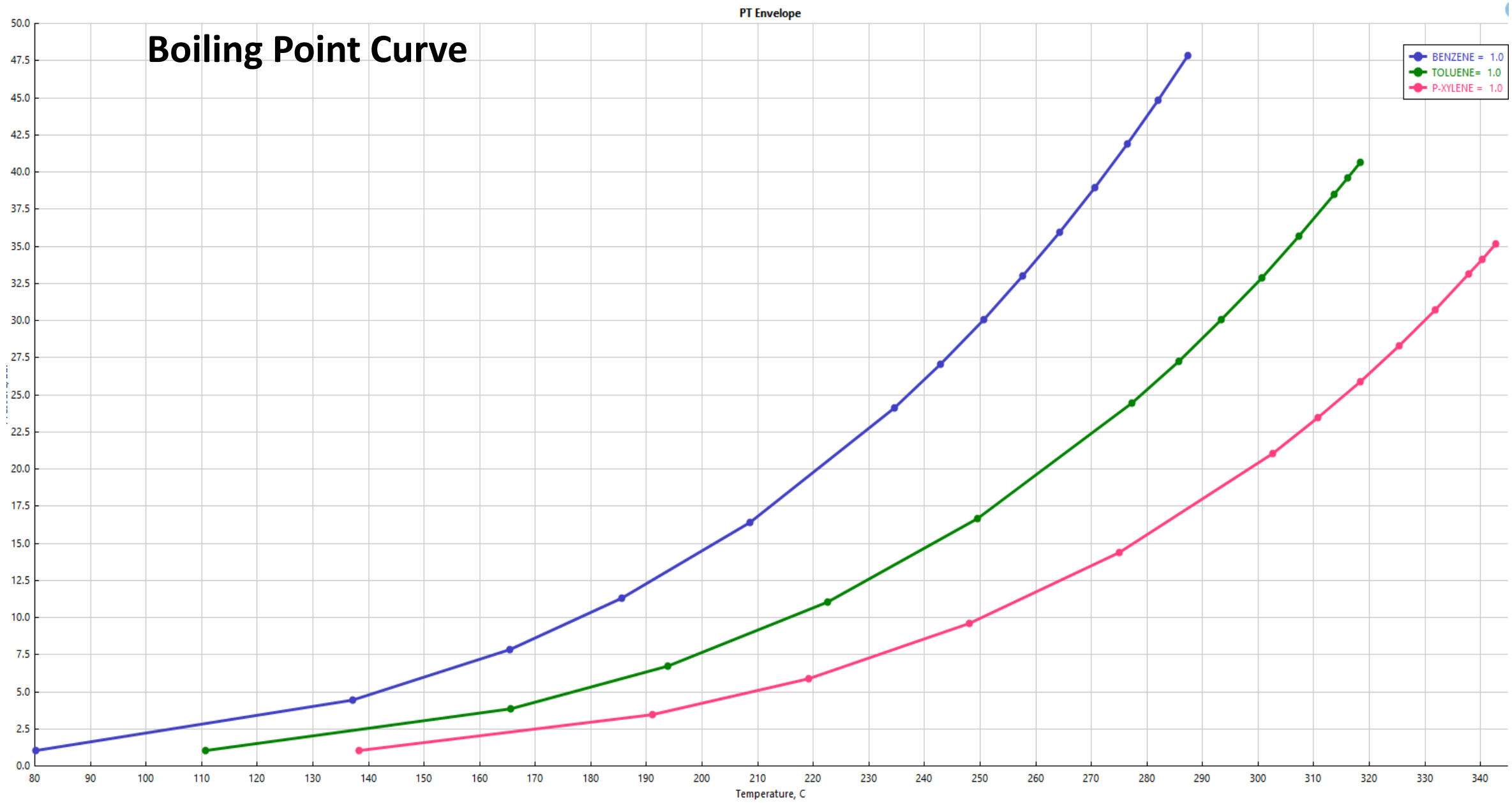


Toluene(119.64 °C)



p-Xylene(147.94 °C)

PT Envelope


PT Envelope
Boiling Point Curve
BENZENE = 1.0
TOLUENE= 1.0
P-XYLENE = 1.0
50.0
47.5
45.0
42.5
40.0
37.5
35.0
32.5
30.0
27.5
25.0
22.5
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320
330
340
Temperature, C

Verification of K values and Relative Volatilities

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	0.215803	0.407234	2.16369
TOLUENE	0.517859	0.595232	0.517859	0.997548
P-XYLENE	0.0749066	0.188965	0.0749066	0.454513

p-xylene

Component	F	X	Y	K
BENZENE	0.407234	0.237485	0.407234	3.79952
TOLUENE	0.517859	0.591038	0.517859	1.94141
P-XYLENE	0.0749066	0.171477	0.0749066	0.967906

- For each simulation, highest K values is for Benzene and lowest is for p-xylene.
- It means Benzene is light key and Toluene is a choice of heavy key.
- No azeotrope is formed in this temperature range.
- Relative Volatility(α) = K of light comp.\K of heavy comp.

K(light component)	1.00707	2.16368	3.79945	
K(heavy component)	0.408843	0.997547	1.94139	
Relative Volatility	2.46321938	2.16900056	1.95707715	2.19643236
				2.18670518

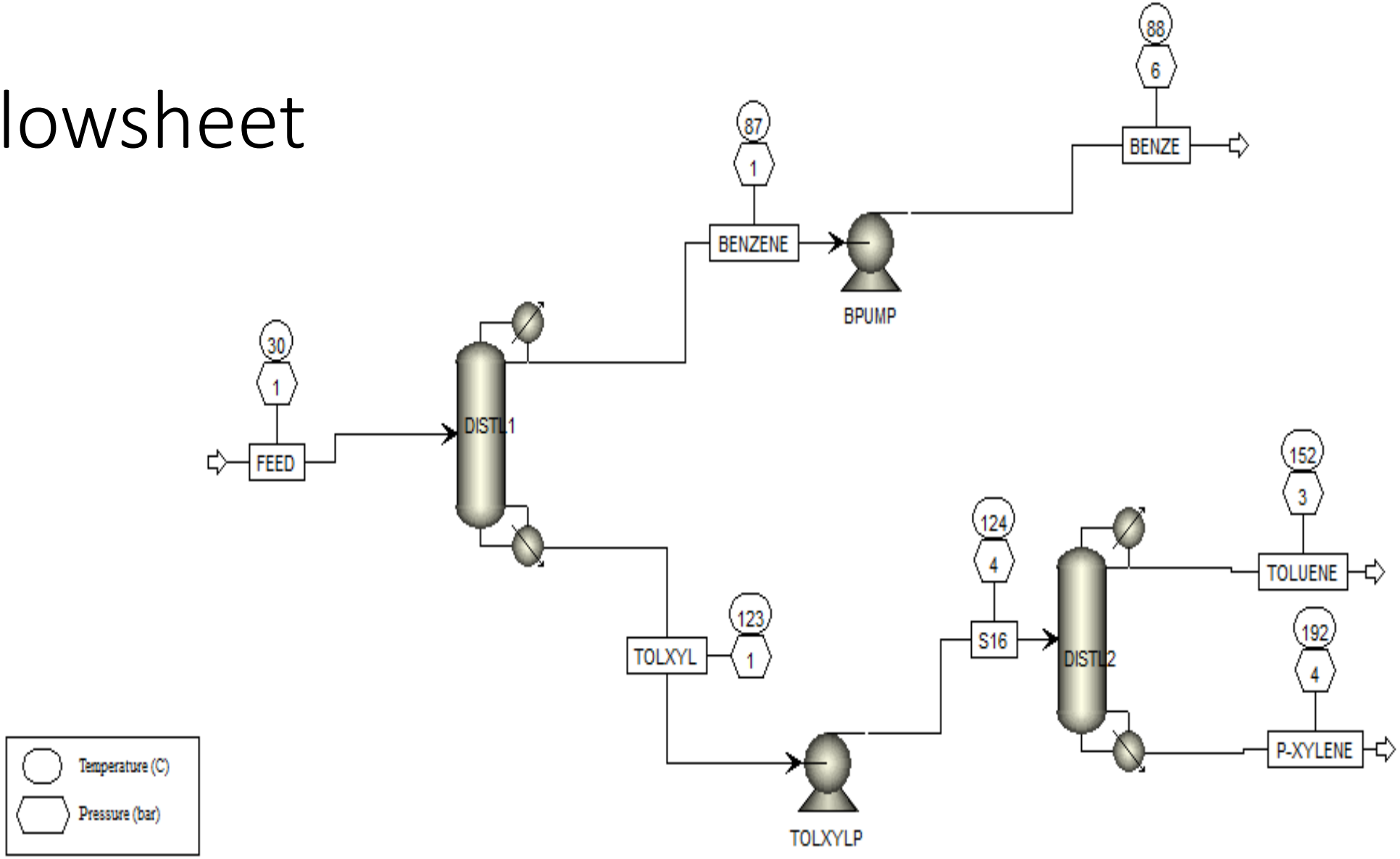
Arithmetic average

Geometric average

Relative Volatility = 2.19
xD = 0.95
xB = 0.03(guess)

Fenske Equation to calculate minimun number of stages: $$N = \frac{\log\left[\left(\frac{X_d}{1-X_d}\right)\left(\frac{1-X_b}{X_b}\right)\right]}{\log \alpha_{avg}}$$ =6.9610076

Main Flowsheet



Results and Stream Results:

Minimum reflux ratio	1.34851954	
Actual reflux ratio	1.68624	
Minimum number of stages	7.93972	
Number of actual stages	15.8794	
Feed stage	9.16466	
Number of actual stages above feed	8.16466	
Reboiler heat duty	163910	Watt
Condenser heat duty	-116052	Watt
Distillate temperature	86.5191	C
Bottom temperature	123.646	C
Distillate to feed fraction	0.402411	
HETP		

	Units	S16	P-XYLENE	TOLUENE	
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	J/kmol	2.66758e+07	1.70686e+07	3.6792e+07	
Mass Enthalpy	J/kg	285820	164522	402130	
Molar Entropy	J/kmol-K	-297016	-337339	-272828	
Mass Entropy	J/kg-K	-3182.39	-3251.56	-2981.95	
Molar Density	kmol/cum	8.21454	6.70675	8.02745	
Mass Density	kg/cum	766.671	695.804	734.455	
Enthalpy Flow	Watt	55719.3	5347.82	65322.1	
Average MW		93.331	103.747	91.4929	
+ Mole Flows	**kmol/hr**	**7.51952**	**1.12793**	**6.39159**	
− Mole Fractions					
BENZENE		0.0403876	3.50623e-06	0.0475142	
TOLUENE		0.834354	0.172561	0.951141	
P-XYLENE		0.125258	0.827435	0.00134433	
+ Mass Flows	**kg/hr**	**701.804**	**117.019**	**584.785**	
+ Mass Fractions					
Volume Flow	l/min	15.2565	2.80297	13.2703	
+ Liquid Phase					
<add properties>					