

Dear Mr. Abbasi,

Our team hopes this note finds you well. Enclosed in the report and detailed analysis of the plant designs built to the specifications of the provided fuel streams TQ1 and K, with special consideration given to stream K. The team examined several set-ups and criteria for reaching the given end goal specifications and believe it is found to be an achievable economic and profitable design. The design makes use of a fired heater and PFR to model the catalytic reformer for a “endothermic reactors” section, followed by Liquid-Liquid Extractors and Reboiled Absorbers for the “extraction section” and distillation columns for the “distillation section” to capture and fractionate the BTX reformat into its separate components.

In the time frame allotted to for the project, designs were created for both the K and TQ1 feeds that met the specification of purity for the BTX reformat stream while also achieving the 99% separation of Benzene, Toluene and p-Xylene in the distillation section as requested. It was predicted that the K feed would lead to a more profitable design, and this was proven in our end result. Additionally, a very pure fraction of hydrocarbons that can be processed into diesel was collected at a very profitable flow rate. The estimates are that in the first year of operation, the revenue after paying for utilities and taxes will be in the hundreds of millions. Our ROR in this model under Kurdish taxes and Iraqi taxes are 15.85% and 12.16%, respectively. It is believed that this project is worth pursuing, but your judgement on the matter will have the final say.

Spring 2021

AICHe Design Project
Abbasi Fuel Refinery Retrofit

April 16, 2021

3. Executive Summary

The goal of this project was to design an efficient plant process meant for the primary reason of removing benzene from the products that will be produced. The design was created with reduced costs and operations in mind while producing an output of a diesel product free of Reformate (BTX). The diesel stream is the most valuable in the process and was optimized as such allowing the sale of the Reformate as a lucrative side product revenue stream.

The design consists of three fixed bed continuous catalytic reformers fed into a vapor-feed separator for the removal of Hydrogen from the newly cracked hydrocarbons. The liquid product is sent to an absorber, which separates the benzene rich diesel from the product. The benzene rich stream enters two liquid-liquid extractors using sulfolane as the solvent to further separate aromatics from the alkanes and washed with water to be separated from the sulfolane. The bottoms product goes into a separator and splitter to recycle the sulfolane back into the system while the benzene goes to a stripper then distillation column for extraction to its 99% purity specification. The diesel streams from the separations made up until this point are summed up and combined to be sold at 99% purity as requested. Factors of safety and environmental concern were considered when sizing the equipment, with an additional 15% psi safety parameter added to the operational pressures of the equipment during costing.

To begin the project at 15% tax an initial investment of \$40 million is needed expecting a payback period of 1.07 years. The expected operating cost was estimated to be \$12 million per year with an expected 15 operators to run a continuous production operation. The NPV of the project is estimated to be \$5.8 billion, with a discounted cash flow rate of 1432% return, and a rate of return of 15.9% for the 30-year expected life of the project. To begin the project at 35% tax an initial investment of \$40 million is needed expecting a payback period of 1.09 years. The NPV of the project is estimated to be \$4.4 billion, with a discounted cash flow rate of 1096% return, and a rate of return of 12.2% for the 30-year expected life of the project. After considering the preliminary design figures, it is recommended the project have consideration for implementation.

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Brief Process Description

Overall, in this process the team simulated two different simulations at a flow rate of 35,000 barrels per day, pressure of 1.2 bar, 70°C, using the UNIFAC LLE NRTL-Ideal fluid package to compare with each other. The two were similarly simulated in HYSYS with only a difference in composition shown In Figure (1). In both simulations the feed streams flow into a pump, P-100, to increase the pressure to 9.2 bar in the stream to allow for optimal reaction conditions before feeding it through a fired heater to PFR-100, recycling it through the fired heater to PFR-101, and recycling it once more through PFR-103. To take advantage of heat integration the stream is fed into a series of heat exchangers that cool the separator stream with the feed streams of Sulfolane and water that are being sent to the Liquid-Liquid extractors, T-100 and T-101. After that, the stream will enter the separator, V-100, to isolate the hydrogen from the hydrocarbons. The hydrogen rich vapor stream is sent to the separator, V-102, after cooling the stream to achieve a better separation and reacquire the hydrocarbons. The liquid hydrocarbon stream is added back into the system into the first absorber column, T-107, along with the bottom stream of the initial separator, V102, that uses a pressure relief valve to match the pressure of the absorber column. The Benzene rich vapor stream from the absorber T-107 is sent through another valve to match the pressure of equipment further downstream while the bottoms stream is collected to converge with the other diesel component streams downstream in the refinery. After proceeding through the first LLE, the top stream is sent to the separator, V-101, to purge the lighter components from the heavier hydrocarbons, with the heavier components collected to be mixed with other diesel streams. The bottom LLE stream goes to the second LLE, T-101, where the bottom stream is purged of water as vapor in the reboiled absorber, T-106, from the Sulfolane where both are recycled back into the system for heat exchange. The top stream of the second LLE, T-101 is sent to the reboiled absorber T-102, for further fractionation of Benzene from heavier components. The bottom stream from this absorber is collected and converged with other diesel streams, and the top is sent to the distillation column, T-108 that produces the reformat stream. The reformat stream then proceeds to distillation column T-103, which collects benzene out of the top stream and sends the toluene and p-Xylene to distillation column T-104, to collect them from the top and bottom streams, respectively.

		crude oil	
		TQ1	K
naphtha proxy components	naphtha % volume of crude	28	20
	specific gravity	0.7308	0.749
	n-decane mol%	77.8	59.7
	cyclohexane mol%	20.6	31.3
	benzene mol%	1.6	9

Figure. (1): Naphthalene Feed Compositions

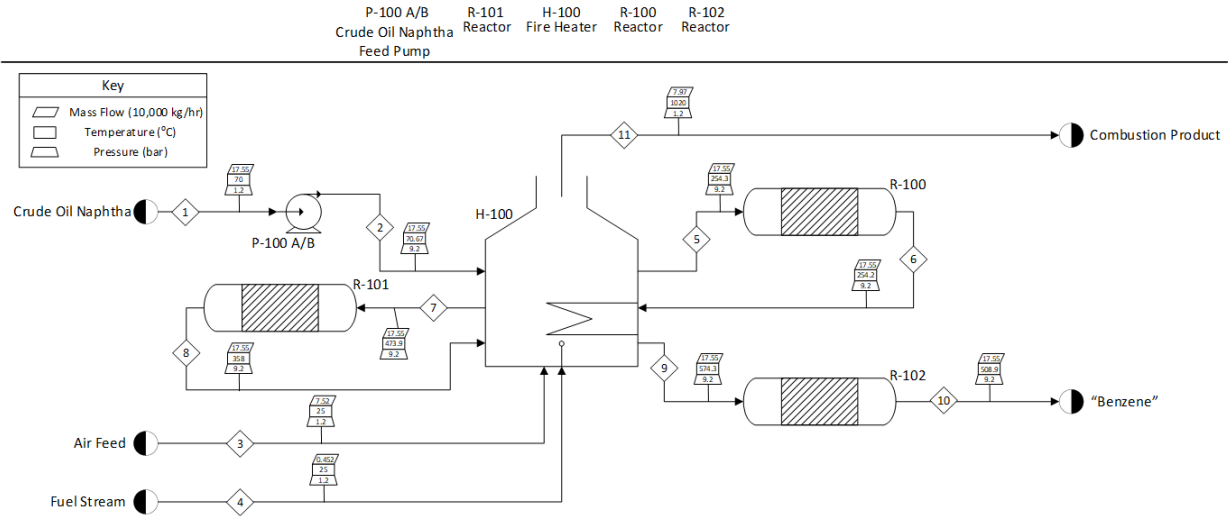


Figure. (2): "K" Feed Reactor Section PFD

Stream		1	2	3	4	5	6
Vapour Fraction		0	0	1	1	0.7902	0.7901
Temperature	°C	70	70.67	25	25	254.3	254.2
Pressure	bar	1.2	9.2	1.2	1.2	9.2	9.2
Molar Flow	kgmole/hr	1483	1483	2603	253	1483	1483
Mass Flow	kg/hr	1.76E+05	1.76E+05	7.52E+04	4.52E+03	1.76E+05	1.76E+05
Liquid Volume Flow	m ³ /hr	233.8	233.8	86.64	14.2	233.8	233.8
Heat Flow	kcal/hr	-7.51E+07	-7.50E+07	0	-4.72E+06	-4.66E+07	-4.66E+07
Stream		7	8	9	10	11	
Vapour Fraction		1	1	1	1	1	
Temperature	°C	473.9	358	574.3	508.9	1020	
Pressure	bar	9.2	9.2	9.2	9.2	1.2	
Molar Flow	kgmole/hr	1483	2323	2323	2872	2871	
Mass Flow	kg/hr	1.76E+05	1.76E+05	1.755E+05	1.76E+05	7.972E+04	
Liquid Volume Flow	m ³ /hr	233.8	252.6	252.6	265.5	95.92	
Heat Flow	kcal/hr	-1.80E+07	-1.80E+07	1.06E+07	1.06E+07	-3.33E+07	

Table. (1): Reactor Section Stream Information

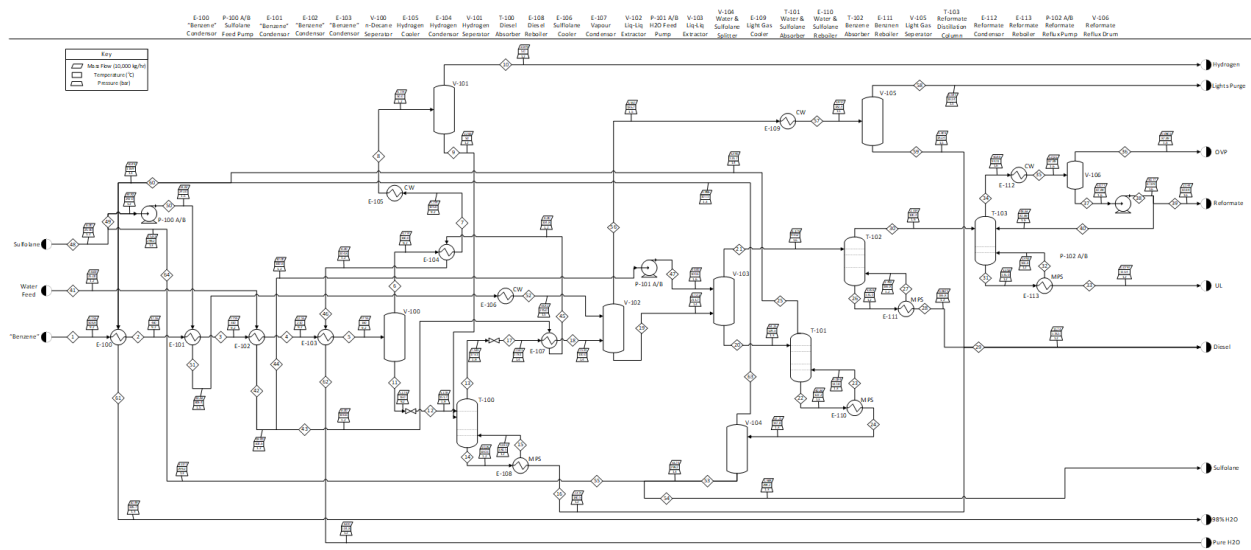


Figure. (3): "K" Feed Extractor Section PFD

Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Vapour Fraction	1	1	1	1	1	1	0.8697	0.8903	0	1	0	0.0987	1	0	1	0	1	0.1247	0.0166	0.0275
Temperature °C	508.9	430	310	210	160	160	105	50	50	160	151.7	173.1	180.5	180.5	180.5	173.1	110	213.7	129.3	
Pressure bar	9.2	9.2	9.2	9.2	9.2	9.2	9.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.2	1.4	1.4	1.4	1.3
Molar Flow kgmole/hr	2872	2872	2872	2872	2872	1850	1850	1850	203	1647	1022	700	1427	901.5	525.1	700	700	3233	8427	
Mass Flow kg/hr	1.76E+05	1.76E+05	1.76E+05	1.76E+05	1.76E+05	4.77E+04	4.77E+04	4.77E+04	2.23E+04	2.55E+04	1.28E+05	1.28E+05	7.53E+04	2.03E+05	1.28E+05	7.47E+07	7.53E+04	7.53E+04	3.74E+05	4.43E+05
Liquid Volume Flow m ³ /hr	265.5	265.5	265.5	265.5	265.5	95.13	95.13	95.13	28.63	66.5	170.4	170.4	97.03	277	1.75	102	97.03	97.03	310.7	372.6
Heat Flow kcal/hr	1.06E+07	1.00E+05	-1.46E+07	-2.83E+07	-3.93E+07	2.82E+06	-7.44E+05	-2.04E+06	-2.89E+06	3.81E+06	-4.21E+07	-4.21E+07	-8.90E+06	-8.34E+07	-4.43E+07	-3.07E+07	-8.90E+06	-1.65E+07	-2.73E+08	-6.42E+08
Stream	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
Vapour Fraction	0.0362	0	1	0	1	0	1	0	0.0152	1	0	1	0	1	1	1	1	1	1	0
Temperature °C	94.52	122.2	137.8	137.8	123.7	131	165.8	165.8	178.5	100.4	90.69	113.4	113.4	94.11	87.89	87.89	87.89	87.89	87.89	87.89
Pressure bar	1.6	1.3	1.3	1.3	1.4	1.2	1.2	1.2	1.2	1.6	1.2	1.2	1.2	1.2	1.6	1.6	1.6	1.6	1.6	1.6
Molar Flow kgmole/hr	357.3	6739	1712	5027	3400	266.8	204.3	62.48	829	295	5494	5487	7.002	6526	6526	13	6526	6526	275	6328
Mass Flow kg/hr	3.18E+04	4.08E+05	3.08E+04	3.78E+05	6.50E+04	3.36E+04	2.49E+04	8657	1.17E+05	2.31E+04	4.88E+05	4.87E+05	796.6	5.09E+05	5.09E+05	9.02E+02	5.09E+05	5.09E+05	2.14E+04	4.86E+05
Liquid Volume Flow m ³ /hr	38.26	337.4	30.91	306.5	66.1	44.95	33.17	11.79	160	26.48	614.2	613.2	1.066	578.2	578.2	1.038	578.2	578.2	24.37	552.8
Heat Flow kcal/hr	-3.25E+05	-5.52E+08	-9.71E+07	-4.35E+08	-1.88E+08	-1.21E+07	-6.07E+06	-3.52E+06	-4.83E+07	5.67E+06	-4.98E+07	-3.33E+06	-2.64E+05	1.36E+08	1.13E+05					
Stream	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
Vapour Fraction	0	0	0	0	0	0.1699	0.258	0	0	0	0.0686	0	0	0	0	0.6457	0.14	1	0	1
Temperature °C	25	100.6	100.6	100.6	104.8	104.8	100.6	25	242	242	306.4	245	299.2	299.2	299.2	186.7	182.4	182.4	182.4	116.9
Pressure bar	1.2	1.2	1.2	1.2	1.2	1.2	1.6	1.2	1.2	1.5	1.5	1.5	1.3	1.3	1.3	1.5	1.5	1.5	1.5	1.3
Molar Flow kgmole/hr	9992	9992	4441	5551	4441	4441	5551	665.7	2814	2814	2814	2809	140.5	2669	280.7	280.7	280.7	39.29	241.4	5618
Mass Flow kg/hr	1.80E+05	1.80E+05	8.00E+04	1.00E+05	8.00E+04	8.00E+04	1.00E+05	8.00E+04	3.38E+05	3.38E+05	3.38E+05	3.38E+05	3.38E+05	1.69E+04	3.21E+05	3.92E+04	3.92E+04	5140	3.40E+04	1.05E+05
Liquid Volume Flow m ³ /hr	180.4	180.4	80.16	100.2	80.16	80.16	100.2	63.14	266.9	266.9	266.9	266.9	266.9	13.32	253.1	53.28	53.28	6.997	46.28	106.1
Heat Flow kcal/hr	-6.80E+08	-6.67E+08	-2.96E+08	-3.70E+08	-2.89E+08	-2.85E+08	-3.70E+08	-7.24E+07	-2.72E+08	-2.72E+08	-2.57E+08	-2.71E+08	-2.61E+08	-1.30E+07	-2.48E+08	-1.45E+07	-1.60E+07	-1.85E+06	-1.41E+07	-3.15E+08
Stream	61	62	63	64																
Vapour Fraction	1	0.5095	1	0																
Temperature °C	326.7	104.8	107.1	299.2																
Pressure bar	1.3	1.2	1.3	1.3																
Molar Flow kgmole/hr	5618	4441	2218	2148																
Mass Flow kg/hr	1.05E+05	8.00E+04	4.00E+04	2.58E+05																
Liquid Volume Flow m ³ /hr	106.1	80.16	40.04	203.8																
Heat Flow kcal/hr	-3.04E+08	-2.74E+08	-1.26E+08	-1.99E+08																

Table. (2): Extractor Section Stream Information

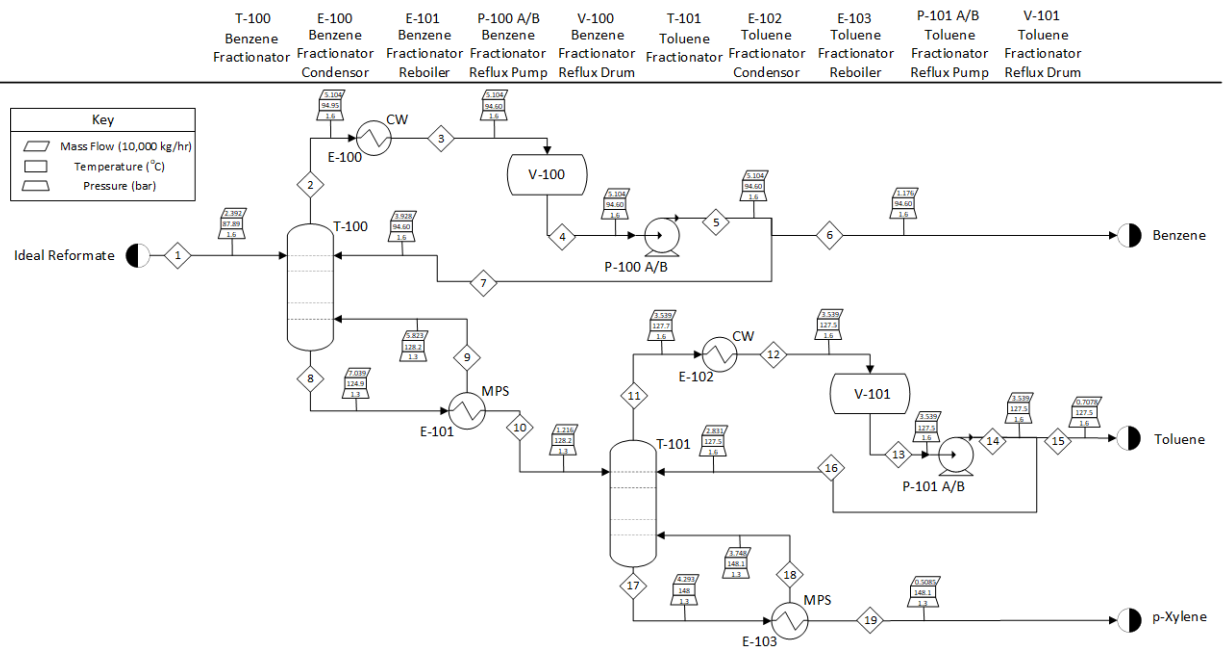


Figure. (4): "K" Feed Distillation Section PFD

Stream		1	2	3	4	5	6	7	8	9	10
Vapour Fraction		0	1	1	1	1	0	0	0	1	0
Temperature	°C	87.89	94.95	94.6	94.6	94.6	94.6	94.6	124.9	128.2	128.2
Pressure	bar	1.6	1.6	1.6	1.6	1.6	1.6	1.6	1.3	1.3	1.3
Molar Flow	kgmole/hr	275	652.2	652.2	652.2	652.2	150.3	501.9	735.9	611.2	124.7
Mass Flow	kg/hr	2.39E+04	5.10E+04	5.10E+04	5.10E+04	5.10E+04	1.18E+04	3.93E+04	7.04E+04	5.82E+04	1.22E+04
Liquid Volume Flow	m ³ /hr	27.35	57.86	57.86	57.86	57.86	13.33	44.53	81.05	67.03	14.02
Heat Flow	kcal/hr	2.37E+06	1.39E+07				2.12E+06	7.07E+06	3.73E+06	8.19E+06	5.18E+05
Stream		11	12	13	14	15	16	17	18	19	
Vapour Fraction		1	1	1	1	0	0	0	1	0	
Temperature	°C	127.7	127.5	127.5	127.5	127.5	127.5	148	148.1	148.1	
Pressure	bar	1.6	1.6	1.6	1.6	1.6	1.6	1.3	1.3	1.3	
Molar Flow	kgmole/hr	384	384	384	384	76.81	307.2	404.5	356.6	47.91	
Mass Flow	kg/hr	3.54E+04	3.54E+04	3.54E+04	3.54E+04	7078	2.83E+04	4.29E+04	3.78E+04	5058	
Liquid Volume Flow	m ³ /hr	40.68	40.68	40.68	40.68	8.135	32.54	49.67	43.79	5.883	
Heat Flow	kcal/hr	5.74E+06				5.53E+05	2.21E+06	1.14E+05	3.13E+06	1.30E+04	

Table. (3): Distillation Section Stream Information

Capital Cost Estimates

a.) Distillation Columns

There exist three distillation columns that are sized and cost in this design. For each column, there are several steps in order to obtain the capital cost estimate. The first step is to size the column and in order to do this the volume was calculated. The second step is to calculate the C_{po} , F_p , and F_m values using Appendix A in the Turton book for stainless steel vertical process vessels. The C_{po} value of the columns was found by using the K values for vertical process vessels and those are provided in the Table (4). The third step of this process is to find the B_1 and B_2 values and these are located in Table (4). Once these numbers are found, the present C_{bm} value can be calculated by multiplying the 2001 value by $(593.6/397)$. A similar process is done in order to calculate the cost of the trays. The first step is to calculate the C_{po} for trays, F_{bm} , and F_q values. The K values required to find the C_{po} for the trays are shown in Table (5). The next step is to calculate the present C_{bm} value for the trays by multiplying the 2001 value by the same value as shown above. The final step in this process is the two C_{bm} values are then added together to get the total capital cost estimate for the distillation columns. For the design, the overall capital cost for distillation columns was \$12,000,000.

K and B Values For Towers	
K1	3.50
K2	0.45
K3	0.11
B1	2.25
B2	1.82

Table. (4): K and B Values for Towers

K Values For Trays	
K1	2.99
K2	0.45
K3	0.40

Table. (5): K Values for Trays

b.) Absorbers

There were three absorbers that are sized and cost in this design. The capital cost of the columns are calculated the exact same way as in the distillation columns section. The only difference is that packing was used instead of trays. To calculate the cost of the packing, several steps were completed. The first step was to calculate the Cpo and Fbm values by using Appendix A in the Turton book for stainless steel vertical process vessels. The K values required to find the Cpo for the packing are shown in Table (7). The next step of this process is to calculate the present Cbm value. The present Cbm value for the trays can be calculated by multiplying the 2001 value by the same value as shown above which is (593.6/397). The final step is the two Cbm values are added together to get the total capital cost estimate for the absorbers. For the design, the overall capital cost for absorbers was \$5,000,000.

K Values For the Tower	
K1	3.50
K2	0.45
K3	0.11

Table. (6): K Values for the Tower

K Values For the Packing	
K1	2.45
K2	0.97
K3	0.01

Table. (7): K Values for the Packing

c.) Pumps

There exist three pumps that were sized and cost in this design. For each pump, there are several steps in order to obtain the capital cost estimate. The first step is to size the column and in order to do this the drive size was calculated. The second step is to calculate the Cpo, Fp, and Fm values using Appendix A in the Turton book for stainless steel centrifugal pumps. The Cpo value of the columns was found by using the K values for centrifugal pumps and the C values for Fp are provided in Table (8). The third step of this process is to find the B1 and B2 values and these are located in Table (8). Once these numbers are found, the present Cbm value can be calculated by multiplying the 2001 value by (593.6/397). A similar process is done in order to calculate the cost of the driver. The first step is to calculate the Cpo for drivers and Fbm values. The K values required to find the Cpo for the drivers are shown in Table (9). The next step is to calculate the present Cbm value for the trays by multiplying the 2001 value by the same value as shown above. The final step in this process is the two Cbm values are then added together to get the total capital cost estimate for the distillation columns. For the design, the overall capital cost for pumps was \$160,000.

C, K, and B Values For the Pumps	
K1	3.39
K2	0.05
K3	0.15
C1	-0.39
C2	0.40
C3	0.00
B1	1.89
B2	1.35

K Values For the Driver	
K1	1.96
K2	1.71
K3	-0.23

Table. (8): C, K, and B Values for the Pumps

Table. (9): K Values for the Driver

d.) Heat Exchangers, Coolers, Reboilers, and Condensers

There exist eighteen heat exchangers that were sized and cost in this design including coolers, reboilers, and condensers. For each heat exchanger, there are several steps in order to obtain the capital cost estimate. The first step is to size the heat exchanger and in order to do this the area was calculated. The second step is to calculate the C_{po} , F_p , and F_m values using Appendix A in the Turton book for stainless steel fixed-tube heat exchangers. The C_{po} value of the columns was found by using the K values for fixed tube heat exchangers and the C values for F_p are provided in Table (10). The third step of this process is to find the B1 and B2 values and these are located in Table (10). Once these numbers are found, the present C_{bm} value can be calculated by multiplying the 2001 value by $(593.6/397)$. For the design, the overall capital cost for heat exchangers was \$7,000,000.

K, C, and B Values For the Heat Exchangers	
K1	4.32
K2	-0.30
K3	0.16
C1	0.04
C2	-0.11
C3	0.08
B1	1.74
B2	1.55

Table. (10): K, C, and B Values for the Heat Exchangers

e.) Reactors

There exist three reactors that were sized and cost in this design. For each reactor, there are several steps in order to obtain the capital cost estimate. The first step is to size the reactor and in order to do this the volume was calculated. The second step is to calculate the Cpo and Fbm values using Appendix A in the Turton book for stainless steel fermenter reactors. The Cpo value of the columns was found by using the K values for fermenter reactors and those are provided in Table (11). Once these numbers are found, the present Cbm value can be calculated by multiplying the 2001 value by (593.6/397). For the design, the overall capital cost for reactors was \$6,000,000.

K Values For the Reactors	
K1	4.11
K2	0.53
K3	0.00

Table. (11): K Values for the Reactors

f.) Fired Heaters

There exists one fired heater that was sized and cost in this design. The fired heaters are simulated as three with the expectation for the streams to recycle through the same, the fired heater was run under the same conditions to allow this. For the fired heater, there are several steps in order to obtain the capital cost estimate. The first step is to size the fired heater and in order to do this the heat duty was calculated. The second step is to calculate the Cpo, Fp, Ft, and Fbm values using Appendix A in the Turton book for stainless steel non-reactive fired heaters. The Cpo value of the columns was found by using the K values for non-reactive fired heaters and those are provided in Table (12). Once these numbers are found, the present Cbm value can be calculated by multiplying the 2001 value by (593.6/397). For the design, the overall capital cost for distillation columns was \$17,000,000.

K and C Values For the Fired Heaters	
K1	7.35
K2	-1.17
K3	0.20
C1	0.13
C2	-0.24
C3	0.1

Table. (12): K and C values for the Fired Heaters

g.) Separators and Liquid-Liquid Extractors

There exist four separators that were sized and cost in this design. For each separator, there are several steps in order to obtain the capital cost estimate. The first step is to size the column and in order to do this the volume was calculated. The second step is to calculate the C_{po} , F_p , and F_m values using Appendix A in the Turton book for stainless steel vertical process vessels. The C_{po} value of the columns was found by using the K values for vertical process vessels and those are provided in Table (13). The third step of this process is to find the B_1 and B_2 values and these are located in Table (13). Once these numbers are found, the present C_{bm} value can be calculated by multiplying the 2001 value by $(593.6/397)$. A similar process is done in order to calculate the cost of the demistifiers. The first step is to calculate the C_{po} for demistifiers, F_{bm} , and F_q values. The K values required to find the C_{po} for the demistifiers are shown in Table (14). The next step is to calculate the present C_{bm} value for the trays by multiplying the 2001 value by the same value as shown above. The final step in this process is the two C_{bm} values are then added together to get the total capital cost estimate for the distillation columns. For the design, the overall capital cost for distillation columns was \$8,000,000.

K and B Values For Towers	
K1	3.50
K2	0.45
K3	0.11
B1	2.25
B2	1.82

Table (13): K and B Values for Towers

K Values For Demistifier	
K1	3.24
K2	0.48
K3	0.34

Table (14): K Values for Demistifier

h.) Total Capital Cost Estimates

The capital costs for each piece of equipment in the design was calculated as mentioned in the capital cost section above. After all of these costs were calculated, they were all added up to obtain the total capital costs which is shown in Table (15). The total capital cost was \$40 million. The total capital costs are also known as the fixed capital investment or FCI.

Total Capital Costs	
Absorbers	2,251,416.62
Distillation Columns	4,269,766.84
Heat Exchangers	6,934,030.50
Seperators	3,386,515.27
Reactors	5,695,834.54
Fired Heaters	16,227,680.79
Pumps	138,126.58
Total Capital Costs	38,903,371.14

Table. (15): Total Capital Costs

Utility Cost Estimates

a.) Pumps

To find the utility cost for a pump, several steps must be followed. Step one is to calculate the hydraulic horsepower which is the flow multiplied by the change in pressure divided by 1715. Step two is to find the brake horsepower which is the hydraulic horsepower divided by the pump efficiency. Step three is to calculate the purchased horsepower which is the brake horsepower divided by the motor efficiency. Once this happens, the final step is to make the necessary conversions to get the final operating cost for the pumps. Once the operating costs were calculated for every pump, they were all added up to get the total operating costs of the pumps. The total operating costs for the pumps was roughly \$30,000.

b.) Heat Exchangers, Coolers, Reboilers, and Condensers

To find the utility cost for a heat exchanger, several steps must be followed. Step one is to calculate the heat duty, the temperature change, and the heat capacity. Once these values are calculated, the \dot{m} value can be found by dividing the heat duty by the change of temperature multiplied by the heat capacity. Step three is to calculate the volumetric flow rate which is the mass flow rate multiplied by 0.002. Once this happens, the final step is to make the necessary conversions to get the final operating cost for the heat exchangers. Once the operating costs were calculated for every heat exchanger, the values were added up to get the total operating costs. Overall, the total operating costs for the heat exchangers was estimated to be \$3,000,000.

c.) Total Utility Costs

Once the utility costs were calculated for the pumps and heat exchangers, they were added up into their own categories as mentioned above in parts a and b. The next step is to

determine the total utility costs. In order to do this, the total utility costs of the pumps are added to the total utility costs of the heat exchangers. The total utility costs are \$3,000,000.

Manufacturing and Operator Costs

Throughout the remainder of this report, manufacturing costs and operating costs will be used as interchangeable terms. This is due to the fact that all operating costs in this project fall under the manufacturing costs umbrella. This includes direct manufacturing costs such as operating labor and utility costs, fixed manufacturing costs such as plant overhead, and general manufacturing costs such as administrative costs, R&D costs, and distribution/selling costs Table (16). Taxes and depreciation were not accounted for in this section and were instead independently accounted for in the cash flow table.

In the design, the cost of manufacturing is \$13,000,000, the utility costs are \$2,800,00, and the operating labor costs are \$1,000,000. The main point of discussion here is the operating labor costs and the cost of manufacturing. These values were achieved using a value of 15 operators at an hourly rate of \$33.25 and a service factor of 0.9589 (8400 hours per year) Table (17-18). This is a very conservative estimate and the plant could be operated with less than this number due to some apparatus overlap. However, the 15 operator estimate was used to ensure any issues could be addressed in the shortest reasonable response time. If the numbers of operators were reduced, it would reduce the costs of operating labor which would, in-turn, reduce the costs of the direct supervisory and clerical labor, laboratory charges, plant overhead, and administrative costs. A reduction in the number of operators would also reduce the cost of manufacturing which would, in-turn, reduce the cost of patents and royalties, research and development, and distribution and selling. The estimated overall total for the manufacturing cost of the design is \$12,000,000.

Manufacturing Costs Table		
Cost Item	Value	Equation
Utility Costs	\$2,707,231.78	CUT
Operating Labor	\$994,767.12	COL
Direct Supervisory and Clerical Labor	\$174,084.25	0.18*COL
Maintenance and Repairs	\$2,334,202.27	0.06*FCI
Operating Supplies	\$350,130.34	0.009*FCI
Laboratory Charges	\$149,215.07	0.15*COL
Patents and Royalties	\$391,446.48	0.03*COM
Total Direct Manufacturing Costs	\$7,101,077.31	Summation
Plant Overhead Costs	\$2,104,816.48	0.708*COL + 0.036*FCI
Depreciation and Taxes	N/A (Handled Separately)	N/A
Total Fixed Manufacturing Costs	\$2,104,816.48	Summation
Administration Costs	\$526,204.12	0.177*COL + 0.009*FCI
Research and Development	\$652,410.81	0.05*COM
Distribution and Selling	\$1,435,303.78	0.11*COM
Total General Manufacturing Costs	\$2,613,918.70	Summation
Total Operating Costs	\$11,819,812.50	Summation

Table. (16): Manufacturing Costs Table

Equipment	Number
HE	9
Towers	6
Compressors	0
Total	15

Table. (17): Operator Equipment

Operator Calculations K Stream	
NOL	3.12
Required #	14.04
Hourly Rate	33.25
Hours per year	29917.81
Cost of Operating	\$994,767.12

Table. (18): Operator Calculations K Stream

Cash Flow Table Analysis

The final expense spreadsheets are calculated taking into key costing parameters, appropriate economic rates, and other relevant factors. The project was evaluated over a thirty-year project life along with an effective tax rate of both 15% and 35% with a hurdle rate of 10%. For depreciation purposes, the plant was evaluated as a refinery and used a 7 year depreciation

life for MACRS depreciation. In the design, the fixed capital investment is \$40,000,000, the operating costs are \$12,000,000 per year, and the product revenue is \$740,000,000 per year. The NPV, DCFROR, payback period, percent worth cost, and ROR were calculated for both 15% and 35% tax and are provided in Tables (19-20).

Results For 15% Tax	
NPV	5,771,048,869.11
DCFROR	1432%
Payback Period	1.07
PWC	150,327,732.60
ROR	15.85

Table. (19): Results for 15% Tax

Results For 35% Tax	
NPV	4,410,605,704.29
DCFROR	1096%
Payback Period	1.09
PWC	150,327,732.60
ROR	12.16

Table. (20): Results for 35% Tax

Sensitivity Analysis

For this design, a product revenue of \$740,000,000, a cost of manufacture of \$12,000,000, and a fixed capital investment of \$40,000,000 were used as base values. Six scenarios were conducted in this sensitivity analysis. The first scenario deals with multiplying the revenue by 0.85 which is the -15% scenario. The tax of 15% and 35% must also be taken into account so there are two different NPV values for this scenario. The NPV with a tax of 15% comes out to be \$5,000,000,000 and the NPV with a tax of 35% comes out to be \$4,000,000,000 respectively. The second scenario involves the normal values that were calculated in the cash flow table section above which is the 0% scenario. The NPV with a tax of 15% comes out to be \$6,000,000,000 and the NPV with a tax of 35% comes out to be \$5,000,000,000 respectively. The final scenario that was conducted was multiplying the revenue by 1.15 which is the +15% scenario. The NPV with a tax of 15% comes out to be \$7,000,000,000 and the NPV with a tax of 35% comes out to be \$5,000,000,000 respectively. The results from these scenarios are shown in Tables (21-26) which include the NPV, DCFROR, payback period, percent worth cost, and ROR. Every scenario shown here at 15% and 35% tax are all valid because they all generate enormous value.

Results For -15% At 15% Tax	
NPV	4,885,980,974.75
DCFROR	1213%
Payback Period	1.08
Percent Worth Cost	150,327,732.60
ROR	13.44

Table. (21): Results for -15% At 15% Tax

Results For -15% At 35% Tax	
NPV	3,733,789,079.20
DCFROR	928%
Payback Period	1.11
Percent Worth Cost	150,327,732.60
ROR	10.31

Table. (22): Results for -15% At 35% Tax

Results For 0% At 15% Tax	
NPV	5,771,048,869.11
DCFROR	1432%
Payback Period	1.07
Percent Worth Cost	150,327,732.60
ROR	15.85

Table. (23): Results for 0% At 15% Tax

Results For 0% At 35% Tax	
NPV	4,410,605,704.29
DCFROR	1096%
Payback Period	1.09
Percent Worth Cost	150,327,732.60
ROR	12.16

Table. (24): Results for 0% At 35% Tax

Results For +15% At 15% Tax	
NPV	6,656,116,763.46
DCFROR	1651%
Payback Period	1.06
Percent Worth Cost	150,327,732.60
ROR	18.27

Table. (25): Results for +15% At 15% Tax

Results For +15% At 35% Tax	
NPV	5,087,422,329.39
DCFROR	1264%
Payback Period	1.08
Percent Worth Cost	150,327,732.60
ROR	14.00

Table. (26): Results for +15% At 35% Tax

Process Safety

a. Inherent Safety Evaluation

For this particular design the safety concepts of minimization and attenuation are most prevalent. The design applies the concept of minimization in low quantities of Sulfolane compared to water, and is used to prevent contamination and adverse effects from high concentration exposure to Sulfolane by recycling what is not used and utilizing that to achieve further separation of benzene from the linear hydrocarbons. As for attenuation, active efforts are made to cool the stream coming from the reaction section before it enters the LLEs so that the Sulfolane does not ignite in the presence of the high temperature stream, and to ensure that hydrocarbons stay in liquid state wherever possible to avoid a gaseous combustion in the event of a leak. Additionally, most of the refinery save for the reaction section is run at atmospheric pressure, which will mitigate the risk of gaseous components flashing unless they happen to flash at atmospheric conditions.

b. Process Safety Management

i. Process hazards

One of the most prevalent hazards is the ignition of the hydrocarbons in the reaction section. In order to break down the naphthalene feed (stream 1) into its constituents and then react along the ways indicated in the problem statement, the naphthalene must be subjected to a high temperature and pressure before entering the reactors. In the event of a leak, gaseous hydrocarbons would flood the surrounding area, reacting with oxygen in the air to combust and causing an explosion. This will be a danger to the workers and the equipment if it comes to pass. Another hazard in this process is Sulfolane exposure. The effects of Sulfolane exposure in humans has had little investigation, but exposure to high concentrations of Sulfolane in animals has shown it to damage the central nervous system and cause conditions such as convulsions and hypothermia, though the effects of lower concentrations are unknown. Another concern of the design is for the water vapor cooling stream that exits at 327 °C and contains roughly 1.2 % hydrocarbons. To recycle the water without buildup of contaminants over time, the stream will need to be treated on or off site before reuse. While none of the components are at a concentration in the stream are above their LELs (see part iii), environmental exposure is a concern. Included below is a table containing OSHA chemical exposure and lethal dose limits and several NFPA diamonds regarding compounds involved in the process. The PEL values were converted from ppm to percentages and it shows that most of the component concentrations in the design are above permissible exposure limits, and in some cases lethal dosage limits. To that end, in the event of a leak of any nature extreme caution must be taken. Short chain linear hydrocarbons (Methane-Pentane) are very flammable, but only somewhat irritable to skin without treatment. Longer linear hydrocarbons (Hexane-Nonane) and cyclohexane are slightly less flammable with the same health hazards. Aromatic hydrocarbons (Benzene, Toluene, p-Xylene) are about as flammable as long linear hydrocarbons, but poses an incapacitation risk on continual exposure.

Component	OSHA Component PEL (%)	OSHA Component LD (%)
Methane	N/A	N/A
Ethane	N/A	N/A
Propane	0.1	0.21
n-Butane	0.08	0.16
n-Pentane	0.1	0.15
n-Hexane	0.05	0.11
n-Heptane	0.05	0.075
n-Octane	0.05	0.1
n-Nonane	N/A	N/A
n-Decane	N/A	N/A
Cyclohexane	0.03	0.13
Benzene	0.0005	0.05
CO ₂	0.5	4
CO	0.005	0.12
Sulfolane	Unknown, range 0.0001-0.0999	Unknown, likely 0.1
Toluene	0.02-0.03	0.05
p-Xylene	0.01	0.09

Table. (27): OSHA Exposure Regulations



Figure. (5): Short Chain Linear Hydrocarbons Safety Diamond



Figure. (6): Long Chain Linear Hydrocarbons and Cyclohexane Safety Diamond



Figure. (7): Aromatic Hydrocarbons Safety Diamond

ii. P&ID of the Major Fractionator

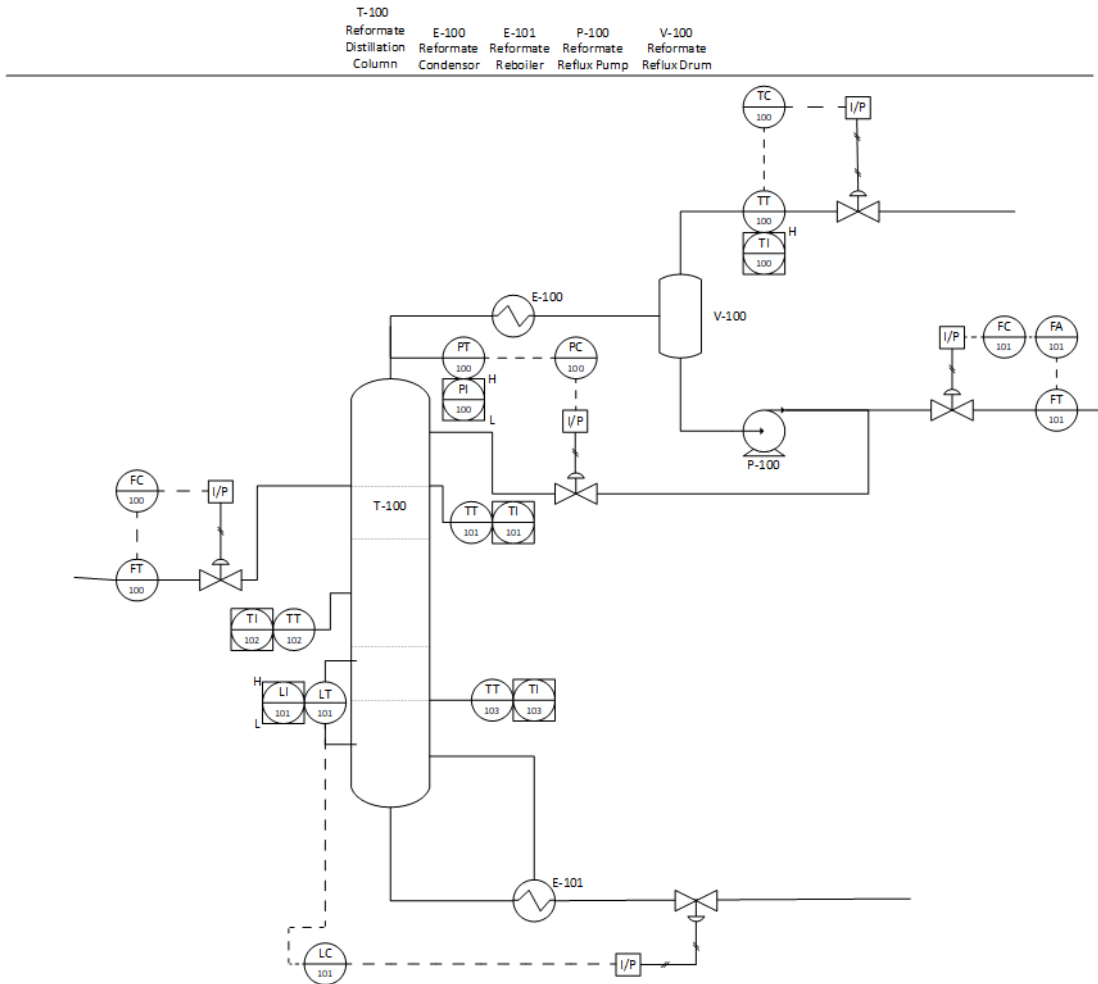


Figure. (8): Major Fractionator P&ID

The aim with the initial flow control loop is to limit the amount of gas entering the column, that way in the event of a leak the rest of the refinery is not fueling the leak continuously. The level control loop near the bottom of the column is designed to shut off flow out of the column to ensure that there is always at least some liquid in the column to become vapor again. The aim with the pressure control loop near the top of the column is to detect the flow of the gas being sent to the condenser and shut off the liquid recycle stream so that no gas backs up the system in the event of gaseous overflow. The aim with the temperature control loop in the overhead vapor stream for the partial condenser is to control the amount of vapor flowing out of the system, and to collect a much more pure product by giving the vapor more time to condense. The aim with the final flow control loop is to analyze the stream composition and, in the event that the stream does not meet the required specification, shut the valve leading to the distillation section and send the liquid back to the column for further processing. The pressure relief designed for the

column is a pressure relief valve with an area of 8.303 cm² that is linked with an onsite flare to safely combust vented gas.

iii. Uncongested Vapor Cloud Deflaguration

Performing a blast radius analysis of a worst case scenario explosion (i.e. maximum efficiency, roughly 10% explosive efficiency) and assuming all contents of the major fractionator vents and combusts with the surrounding atmosphere it is found that around 2225 m from the explosion is the minimum “safe distance” at which whatever damage may be caused to structures is not considered serious. Around 1675 m away from the explosion, structural damage considered minor can occur. Between 1362 m and 687 m away from the explosion, more noticeable structural damage can occur; roughly 971 m away from the explosion, minor damage to house structures occurs and around 687 m away partial demolition of houses occurs. It is around this point that human damage becomes more and more likely, and the circumstances only become deadlier the closer a human is to the initial explosion. Included below are the components that would likely become gaseous and react with the air explosively, along with their respective Lower Explosive Limit and Upper Explosive Limit. Concentrations below and above these values mean something is too “poor” to burn or too “rich” to burn, respectively. A majority of the components flowing into the major fractionator are below their respective LELs save for Benzene, Toluene and p-Xylene which are above their respective UELs. Initially, no explosion will occur, but as the Benzene, Toluene and p-Xylene diffuse through the outside air they will reach a concentration that will ignite in the air readily, as well as inflict their harmful exposure effects on unprotected individuals in the vicinity of the leak.

Component	Component LEL (%)	Component UEL (%)
Ethane	3	12.5
Propane	2.1	9.5
n-Butane	1.8	8.4
n-Pentane	1.5	7.8
n-Hexane	1.1	7.5
n-Heptane	1.05	6.7
n-Octane	1	6.5
n-Nonane	0.8	2.9
n-Decane	N/A	N/A
Cyclohexane	1.3	8.4
Benzene	1.3	7.9
H2O	N/A	N/A
Toluene	1.1	8
p-Xylene	1.1	7

Table. (28): LEL and UEL concentrations for compounds Present in Major Fractionator

c. Safety Summary

While impossible to completely eliminate the risk from the operation of this design (or any design proposed for that matter), the findings listed in this section are showing that the design is relatively safe to operate if all safety precautions with equipment and chemicals are followed. Of particular note is the harmful effects of gaseous benzene exposure: inhalation will cause irritation of the respiratory tract and damage the nervous system, and long term exposure will lead to dry, red and cracked skin, while some more immediate effects are dizziness to eventual unconsciousness. To that effect, PPE necessary to ensure the health of the workers would include eye protection (safety goggles) and skin protection (long sleeves, long pants, gloves, closed toe shoes) while dealing with Benzene in liquid form and respiratory protection (breathing masks) when dealing with it in gaseous form. In the event of a gas leak from the major fractionator, all personnel should take precautions to avoid breathing in the gas and evacuating to a safe distance if the leak cannot be contained. Safety systems are in place to avoid an explosion, but they are not foolproof, and personnel safety should be paramount; machinery can be replaced, lives cannot.

Conclusions

This design at a 15% tax rate is more economically attractive than at a 35% tax rate. In terms of NPV, the design at a 15% tax rate is the best option with an NPV of roughly 5.8 billion dollars while the design at a 35% tax rate is roughly 4.5 billion dollars. In terms of payback period, the design with a 15% tax rate is more advantageous with a period of 1.07 years while the design with a 35% tax rate has a period of 1.09 years. Even at the worst case scenario examined, both designs are extremely profitable. Changes in the product revenue have the largest impact of the NPV of the project as seen in the sensitivity analysis. Therefore, these values should be treated with the most importance for any future economic analyses. Given these analyses show economically favorable in either case the project is recommended for consideration.

The design was successful and able to meet all product specifications of 99% required by the problem statement. In creating the design, we noticed the inability to properly extract a pure gasoline product and found that the diesel stream approach was much more lucrative, especially in the K stream. The biggest revenue detractor was the cost of Sulfolane so efforts into implementing recycling was the biggest factor considered besides optimizing the recovery of the heavier component streams.

Assumptions

In designing the plant there were a few assumptions made and some liberties taken during the process. For the assumptions made it was found that the HYSYS binary coefficients used in the UNIFAC LLE NRTL-Ideal fluid package. Literature points to the values being overly generalized in practice with a value disparity of -14253.3 for the Aij Sulfolane-benzene binary interaction coefficients given using the value from Figure (9) below. When changing the coefficients manually in the value table, the simulation changes the properties in the first liquid-

liquid extractor dramatically. The streams exiting the first LLE, T-100, converge to be full liquid where the current simulation shows vapor to be the prevalent phase for the top production stream. This leads to the assumption the thermodynamic calculations may not be completely accurate for the process design provided.

Table 2. NRTL binary interaction parameters for the system Octane-Benzene-Sulfolane* at 298.15 K

i	j	a_{ij} (K)		
		Initial guess	Regressed parameters	
			Without closure equations	With closure equations
Octane	Benzene	-545.34	-491.187	-467.597
Benzene	Octane	857.45	878.718	878.496
Benzene	Sulfolane	849.32	839.916	847.876
Sulfolane	Benzene	-534.04	-568.212	-545.395
Octane	Sulfolane	1168.85	1211.450	1202.190
Sulfolane	Octane	1188.28	1196.860	1155.020
rmsd		2.6019	0.8523	0.8044

*Experimental LLE data from Lee and Kim [1995].

Figure. (9): NRTL Binary Interaction Parameters

Concerns

There was an oversight in the design where the Sulfolane recycle stream gives two flow values at the same recycle node. This led to miscalculations when converging the process and has led to material and energy balances being unequal. This also led to an instance of having a vapor phase stream of Sulfolane going into the pump that can easily be fixed with an additional heat exchanger before it enters back into the system.

From what is typical in the industry a treatment plant or distillation column which is a costly piece of equipment used to separate water from Sulfolane where aspen allows for the use of a splitter. The concern in using this piece of equipment is the fact that the node does not consider the phase of the components and generalizes the separation process and energy requirements, possibly leading to inaccuracies for the flows and energy balance of the Sulfolane and water streams.

To simulate a divided wall column in HYSYS requires a rigorous trial and error process and the feasible implementation requires a standalone file to properly implement due to the recycle stream calculations impeding calculations for the main equipment that lead to errors. To estimate the flows for the initial simulation a short-column configuration is typically done with an un-ideal stream made of multiple waste components which can be shown in Figure (10). Once this is done the stream values can be used as estimations for the distillation columns that would further simulate the process with ample amounts of recycle and purge streams as shown in Figure (11). It showed to be a very challenging process to implement since it was implied an ideal stream is allowed to be used for calculation for the flow given the addition of p-Xylene and

Toluene in a ratio but not necessary. Overall, the process is feasible however due to the assumption that the feed in this case are splits of compositionally pure Benzene, Toluene, and p-Xylene the benefits would not be an effective representation of its purpose in the current simulated conditions.

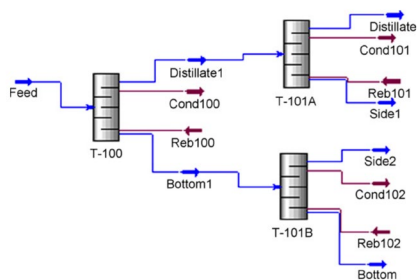


Figure. (10): HYSYS Short Column Example

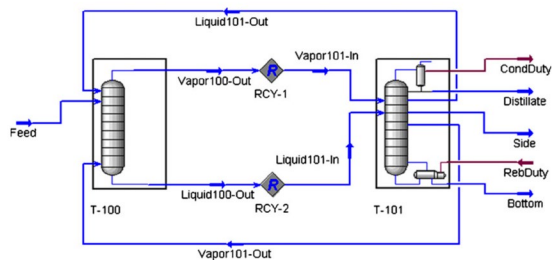


Figure. (11): HYSYS Divided Wall Column

Appendix

a. Reactor Train Detail

The reactor section of the design includes a pump, fired heater, and three fixed bed catalytic reactors. The pump is used to pressurize the feed stream to 9.2bar in order to optimize the conversion of cyclohexane to linear hydrocarbons in the reactors before it sees the extractor section of the process. The fired heater was assumed to run at 50% as it was found in literature to range from 30-80% with atmospheric pressure feeds. Though there was consideration to include a catalyst cost it was found that at 1.0 void fraction the process did not require the calculation and had within a 3% conversion differential of what was believed to have been the right parameters for the catalyst when implemented.

The specific range of temperature for the cracking to heavier hydrocarbons to reduce the conversion to lighter components. The lighter components produced were minute in comparison to the more lucrative diesel components and required more cooling than was feasible while requiring more equipment for acceptable separation. The reactor section was run at 9.2 bar under isobaric conditions for optimal cracking for the design. This is allowable due to a 5% pressure drop being neglected in most modeling simulations for industrial sized cases. To model the reaction for this section the following kinetic parameters used for the conversion rate equations applied in the simulation can be found in Table (26), and Figure (12) below. The “Reaction 1” equation is for cyclohexane dehydrogenation, “Reaction 2” is the kinetics for cyclohexane cracking, “Reaction 3” corresponds with the reaction kinetics for n-Decane cracking, and “Reaction 4” is the kinetics for cyclohexane cyclization.

The project design neglects the use of the Hydrogen recycle stream given in the project statement provided as it was found to lower the effective yield of the product dramatically and introduced complexity. To negate completely ignoring the stream entirely it was cooled and separated at relatively high efficiency from the hydrocarbons that re-enter with the product flow while purging the Hydrogen into the atmosphere. Although the stream is 80% hydrogen there is still a noticeable amount of hydrocarbon materials in the stream and would need to be stored or sent off to be treated to environmental standards.

K Stream Kinetic Parameters				
Forward:	Reaction 1	Reaction 2	Reaction 3	Reaction 4
A	9.4928×10^{13}	3.6704×10^{21}	3.6704×10^{21}	3.33674×10^{19}
E [kJ/kmol]	160,506.40	287,756.80	287,756.80	275,285.80
Reverse:				
A'	8.2728×10^{-4}			4.19816×10^{21}
E' [kJ/kmol]	-52,170.40			312,237.90

Table (29): Kinetic Parameters

$$\begin{aligned}
 \text{rate} &= 9.4928 \times 10^{13} e^{\frac{-160506.4}{8.314T}} P_{C_6H_{12}} - 8.2728 \times 10^{-4} e^{\frac{52170.4}{8.314T}} P_{C_6H_6} P_{H_2}^3 & \text{rate} &= 3.6704 \times 10^{21} e^{\frac{-287756.8}{8.314T}} P_{C_6H_{12}} \\
 \text{rate} &= 3.6704 \times 10^{21} e^{\frac{-287756.8}{8.314T}} P_{C_{10}H_{22}} & \text{rate} &= 3.33674 \times 10^{19} e^{\frac{-275285.8}{8.314T}} P_{C_6H_{12}} P_{H_2} - 4.19816 \times 10^{21} e^{\frac{-312237.9}{8.314T}} P_{C_6H_{12}}
 \end{aligned}$$

$\text{rate} \equiv \text{kmol} / (\text{m}^3 \text{hr}), \quad P \equiv \text{MPa}, \quad T \equiv \text{Kelvin}$

Figure. (12): Kinetic Equations for Reactions [1-4]

Name	K	MS1	Q1
Vapour	0.0000	0.0000	<empty>
Temperature [C]	70.00	70.67	<empty>
Pressure [bar]	1.200	9.200	<empty>
Molar Flow [kgmole/h]	1483	1483	<empty>
Mass Flow [kg/h]	1.755e+005	1.755e+005	<empty>
Std Ideal Liq Vol Flow [m3/h]	233.8	233.8	<empty>
Molar Enthalpy [kcal/kgmole]	-5.063e+004	-5.059e+004	<empty>
Molar Entropy [kJ/kgmole-C]	115.4	133.1	<empty>
Heat Flow [kcal/h]	-7.510e+007	-7.504e+007	6.297e+004

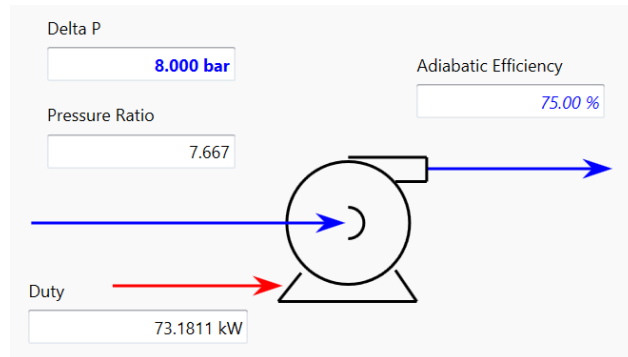


Figure. (13): Pump Specifications for P-100:
Streams K, and MS1: Reactions section PFD stream equivalent 1, and 2

Tube Dimensions	
Total Volume	15.71 m ³
Length	5.000 m
Diameter	2.000 m
Number of Tubes	1
Wall Thickness	5.000e-003 m

Name	MS2	MS3
Vapour	0.7902	0.7901
Temperature [C]	254.3	254.2
Pressure [bar]	9.200	9.200
Molar Flow [kgmole/h]	1483	1483
Mass Flow [kg/h]	1.755e+005	1.755e+005
Std Ideal Liq Vol Flow [m ³ /h]	233.8	233.8
Molar Enthalpy [kcal/kgmole]	-3.144e+004	-3.144e+004
Molar Entropy [kJ/kgmole-C]	315.2	315.2
Heat Flow [kcal/h]	-4.663e+007	-4.663e+007

	MS2	MS3
Ethane	0.0000	0.0000
Propane	0.0000	0.0000
n-Butane	0.0000	0.0000
n-Pentane	0.0000	0.0000
n-Hexane	0.0000	0.0000
n-Heptane	0.0000	0.0000
n-Octane	0.0000	0.0000
n-Nonane	0.0000	0.0000
n-Decane	0.5970	0.5969
Cyclohexane	0.3130	0.3129
Benzene	0.0900	0.0900
Hydrogen	0.0000	0.0001

Figure. (14): R-100 Sizing, Properties and Composition:
Streams MS2, and MS3: Reactions section PFD stream equivalent 5, and 6

Tube Dimensions	
Total Volume	157.1 m ³
Length	5.000 m
Diameter	2.000 m
Number of Tubes	10
Wall Thickness	5.000e-003 m

Name	MS4	MS5
Vapour	1.0000	1.0000
Temperature [C]	473.9	358.0
Pressure [bar]	9.200	9.200
Molar Flow [kgmole/h]	1483	2323
Mass Flow [kg/h]	1.755e+005	1.755e+005
Std Ideal Liq Vol Flow [m ³ /h]	233.8	252.6
Molar Enthalpy [kcal/kgmole]	-1.215e+004	-7761
Molar Entropy [kJ/kgmole-C]	437.0	306.8
Heat Flow [kcal/h]	-1.803e+007	-1.803e+007
	MS4	MS5
Methane	0.0000	0.0000
Ethane	0.0000	0.0000
Propane	0.0000	0.0000
n-Butane	0.0000	0.0000
n-Pentane	0.0000	0.0000
n-Hexane	0.0000	0.0000
n-Heptane	0.0000	0.0000
n-Octane	0.0000	0.0000
n-Nonane	0.0000	0.0000
n-Decane	0.5969	0.3812
Cyclohexane	0.3129	0.0793
Benzene	0.0900	0.1780
Hydrogen	0.0001	0.3615

Figure. (15): R-101 Sizing, Properties and Composition: Streams MS4, and MS5: Reactions section PFD stream equivalent 7, and 8

Tube Dimensions	
Total Volume	1963 m ³
Length	10.00 m
Diameter	5.000 m
Number of Tubes	10
Wall Thickness	5.000e-003 m

Name	MS6	MS7
Vapour	1.0000	1.0000
Temperature [C]	574.3	508.9
Pressure [bar]	9.200	9.200
Molar Flow [kgmole/h]	2323	2872
Mass Flow [kg/h]	1.755e+005	1.755e+005
Std Ideal Liq Vol Flow [m ³ /h]	252.6	265.5
Molar Enthalpy [kcal/kgmole]	4559	3687
Molar Entropy [kJ/kgmole-C]	376.7	320.9
Heat Flow [kcal/h]	1.059e+007	1.059e+007

	MS6	MS7
Methane	0.0000	0.0034
Ethane	0.0000	0.0034
Propane	0.0000	0.0034
n-Butane	0.0000	0.0034
n-Pentane	0.0000	0.0034
n-Hexane	0.0000	0.0007
n-Heptane	0.0000	0.0025
n-Octane	0.0000	0.0025
n-Nonane	0.0000	0.0025
n-Decane	0.3812	0.2971
Cyclohexane	0.0793	0.0000
Benzene	0.1780	0.2078
Hydrogen	0.3615	0.4702
Nitrogen	0.0000	0.0000
Oxygen	0.0000	0.0000
CO ₂	0.0000	0.0000
H ₂ O	0.0000	0.0000
CO	0.0000	0.0000
SULFOLANE	0.0000	0.0000
Toluene	0.0000	0.0000
o-Xylene	0.0000	0.0000
m-Xylene	0.0000	0.0000
p-Xylene	0.0000	0.0000

Figure. (16): R-102 Sizing, Properties and Composition:
Streams MS6, and MS7: Reactions section PFD stream equivalent 9, and 10

- Model Selection		Steady State Parameters				
Steady State model: Simple fired heater		Efficiency:	50.00			
		Excess Air Percent:	10.00			
Name	MS1	AF1	FS1	MS2	CP2	
Vapour	0.0000	1.0000	1.0000	0.7902	1.0000	
Temperature [C]	70.6676	25.0000	25.0000	254.2520	986.3708	
Pressure [bar]	9.200	1.200	1.200	9.200	1.200	
Molar Flow [kgmole/h]	1483.3143	2707.6208	251.1708	1483.3143	2973.3887	
Mass Flow [kg/h]	175500.0031	78223.5462	4489.3624	175500.0031	82712.9086	
LiqVol Flow [m3/h]	233.7579	90.1227	14.1000	233.7579	99.3372	
Molar Enthalpy [kcal/kgmole]	-5.059e+004	0.0000	-1.867e+004	-3.144e+004	-1.113e+004	
Molar Entropy [kJ/kgmole-C]	133.1	188.8	223.3	315.2	234.6	
Heat Flow [kcal/h]	-7.5037e+07	0.0000e-01	-4.6894e+06	-4.6635e+07	-3.3092e+07	
	MS1	AF1	FS1	MS2	CP2	
Methane	0.0000	0.0000	0.9130	0.0000	0.0000	
Ethane	0.0000	0.0000	0.0500	0.0000	0.0000	
Propane	0.0000	0.0000	0.0180	0.0000	0.0000	
n-Butane	0.0000	0.0000	0.0100	0.0000	0.0000	
n-Pentane	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Decane	0.5970	0.0000	0.0000	0.5970	0.0000	
Cyclohexane	0.3130	0.0000	0.0000	0.3130	0.0000	
Benzene	0.0900	0.0000	0.0000	0.0900	0.0000	
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	
Nitrogen	0.0000	0.7800	0.0030	0.0000	0.7105	
Oxygen	0.0000	0.2200	0.0000	0.0000	0.0182	
CO2	0.0000	0.0000	0.0060	0.0000	0.0940	
H2O	0.0000	0.0000	0.0000	0.0000	0.1772	

Figure. (17): H-100 Properties and Composition:

Streams MS1, AF1, FS1, MS2, and CP: Reactions section PFD stream equivalent 2,3,4,5,& 11

Name	MS3	Air_Feed-2	Fuel_Stream-2	MS4	CP3
Vapour	0.7901	1.0000	1.0000	1.0000	1.0000
Temperature [C]	254.2395	25.0000	25.0000	473.8852	986.3708
Pressure [bar]	9.200	1.200	1.200	9.200	1.200
Molar Flow [kgmole/h]	1483.4776	2726.8238	252.9521	1483.4776	2994.4765
Mass Flow [kg/h]	175500.0030	78778.3231	4521.2019	175500.0030	83299.5250
LiqVol Flow [m3/h]	233.7616	90.7618	14.2000	233.7616	100.0417
Molar Enthalpy [kcal/kgmole]	-3.144e+004	0.0000	-1.867e+004	-1.215e+004	-1.113e+004
Molar Entropy [kJ/kgmole-C]	315.2	188.8	223.3	437.0	234.6
Heat Flow [kcal/h]	-4.6635e+07	0.0000e-01	-4.7226e+06	-1.8031e+07	-3.3327e+07

	MS3	Air_Feed-2	Fuel_Stream-2	MS4	CP3
Methane	0.0000	0.0000	0.9130	0.0000	0.0000
Ethane	0.0000	0.0000	0.0500	0.0000	0.0000
Propane	0.0000	0.0000	0.0180	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0100	0.0000	0.0000
n-Pentane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Decane	0.5969	0.0000	0.0000	0.5969	0.0000
Cyclohexane	0.3129	0.0000	0.0000	0.3129	0.0000
Benzene	0.0900	0.0000	0.0000	0.0900	0.0000
Hydrogen	0.0001	0.0000	0.0000	0.0001	0.0000
Nitrogen	0.0000	0.7800	0.0030	0.0000	0.7105
Oxygen	0.0000	0.2200	-0.0000	0.0000	0.0182
CO2	0.0000	0.0000	0.0060	0.0000	0.0940
H2O	0.0000	0.0000	0.0000	0.0000	0.1772

Figure. (18): H-101 Properties and Composition:
Streams MS3 and MS4: Reactions section PFD stream equivalent 6, and 7

Name	MS5	Air_Feed-3	Fuel_Stream	MS6	CP1
Vapour	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature [C]	357.9522	25.0000	25.0000	574.2684	1020.4783
Pressure [bar]	9.200	1.200	1.200	9.200	1.200
Molar Flow [kgmole/h]	2323.1428	2602.8773	252.9521	2323.1428	2870.5300
Mass Flow [kg/h]	175499.4685	75197.4902	4521.2019	175499.4685	79718.6921
LiqVol Flow [m3/h]	252.6488	86.6363	14.2000	252.6488	95.9162
Molar Enthalpy [kcal/kgmole]	-7761	0.0000	-1.867e+004	4559	-1.162e+004
Molar Entropy [kJ/kgmole-C]	306.8	188.8	223.3	376.7	235.3
Heat Flow [kcal/h]	-1.8031e+07	0.0000e-01	-4.7226e+06	1.0591e+07	-3.3345e+07
	MS5	Air_Feed-3	Fuel_Stream	MS6	CP1
Methane	0.0000	0.0000	0.9130	0.0000	0.0000
Ethane	0.0000	0.0000	0.0500	0.0000	0.0000
Propane	0.0000	0.0000	0.0180	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0100	0.0000	0.0000
n-Pentane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000
n-Decane	0.3812	0.0000	0.0000	0.3812	0.0000
Cyclohexane	0.0793	0.0000	0.0000	0.0793	0.0000
Benzene	0.1780	0.0000	0.0000	0.1780	0.0000
Hydrogen	0.3615	0.0000	0.0000	0.3615	0.0000
Nitrogen	0.0000	0.7800	0.0030	0.0000	0.7075
Oxygen	0.0000	0.2200	-0.0000	0.0000	0.0095
CO2	0.0000	0.0000	0.0060	0.0000	0.0981
H2O	0.0000	0.0000	0.0000	0.0000	0.1849

Figure. (19): H-102 Properties and Composition:
Streams MS5 and MS6: Reactions section PFD stream equivalent 8 and 9

Equipment	Base Capital Cost [\$]	Utility Cost [\$/year]
Pumps		
P-100	132242.75	28537.89
Fired Heater		
FH-101	16227680.79	41394.3
PFR		
PFR-101	329316.65	N/A
PFR-102	1116651.14	N/A
PFR-103	4249866.76	N/A
Costs	22055758.09	69932.19
Total	22125690.28	

Table. (30): R & H Capital and Utility Costs

b. Extractor Section Detail

In the Extractor section of the design there are 4 separators used to purge lighter components, 2 pumps to get streams up to column pressure, 3 absorbers for benzene or Sulfolane separation, and a distillation column to produce the reformat product. In the extractor section the most considered factor was controlling the flows of Sulfolane needed in order to extract the benzene from the heavier hydrocarbons from the first LLE and water fed to the second LLE to wash the Benzene of Sulfolane. Running a 4:1 ratio of Sulfolane to the product molar flow was best for separation while minimizing the cost of Sulfolane being the goal due to its high utility cost. To save on these costs a recycle stream was implemented with a 5% purge stream saving an

estimated 700,000,000 [\$/year]. It was found however, that the design has a flaw in the flow rates leading to a generalized estimate. It was discovered that increasing the number of trays, while lowering the temperature and pressure in the distillation column allowed for better separation of Benzene into the reformate stream for higher purity. The water vapor streams from the Sulfolane stream separation process were used for cooling the outgoing reactor stream to a notable degree.

Equipment	Base Capital Cost [\$]	Utility Cost [\$/year]
Pumps		
P-102	14069.02	1221.97
P-103	11646.27	611.74
Separators		
V-100	6669662.79	N/A
V-101	131217.21	N/A
V-102	210578.86	N/A
X-100	879237.11	N/A
Costs	7916411.26	1833.71
Total	7918244.97	

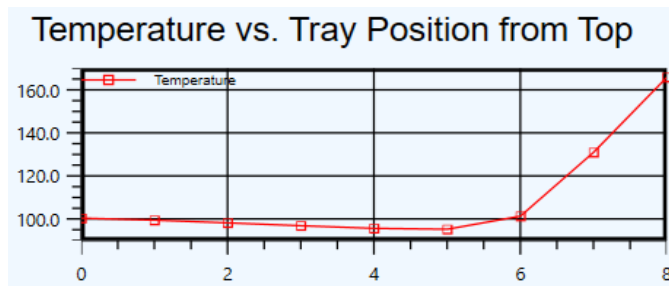
Table. (31): Pumps and Separators Capital and Utility Costs

Equipment	Base Capital Cost [\$]	Utility Cost [\$/year]	Operator Cost [\$/year]
Heat Exchangers			
E-100	177334.00	167145.15	
E-101	227903.61	203313.29	
E-103	181014.75	669671.13	
E-104	425766.10	669619.79	
E-105	347482.78	59677.28	
E-106	357787.91	111595.99	
E-107	258619.73	210445.14	
E-108	158327.91	46168.40	
E-109	994766.44	676550.74	
Costs	3129003.23	2814186.91	596860.27
Total	6540050.41		

Table. (32): Heat Exchanger Costs

Equipment	Base Capital Cost [\$]	Utility Cost [\$/year]	Operator Cost [\$/year]
Absorbers			
T-102	673288.54	13444.84	
T-106	1815637.85	15567.23	
T-107	3323366.26	71418.96	
Distillation Columns			
T-108	12139880.44	365627.48	
Costs	17952173.09	466058.51	265271.23
Total	18683502.83		

Table. (33): Extractor Section Column Costs

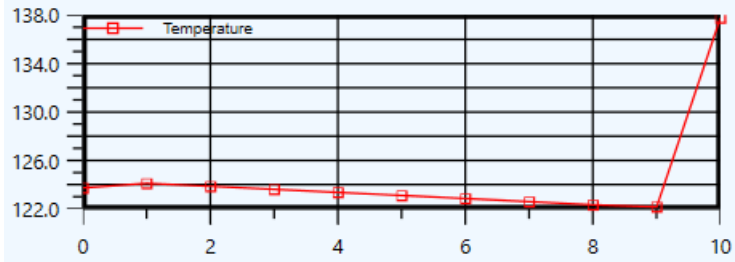


Name	S19.1 @COL3	S22 @COL3	S23 @COL3
Vapour	0.0362	1.0000	0.0000
Temperature [C]	94.52	100.4	165.8
Pressure [bar]	1.600	1.600	1.200
Molar Flow [kgmole/h]	357.5	295.0	62.48
Mass Flow [kg/h]	3.179e+004	2.314e+004	8657
Std Ideal Liq Vol Flow [m3/h]	38.26	26.48	11.79
Molar Enthalpy [kcal/kgmole]	-909.0	1.922e+004	-5.639e+004
Molar Entropy [kJ/kgmole-C]	2.982	14.08	360.0
Heat Flow [kcal/h]	-3.250e+005	5.670e+006	-3.523e+006

	S19.1	S22	S23
Methane	0.0000	0.0000	0.0000
Ethane	0.0002	0.0002	0.0000
Propane	0.0005	0.0006	0.0000
n-Butane	0.0017	0.0021	0.0000
n-Pentane	0.0036	0.0043	0.0000
n-Hexane	0.0011	0.0013	0.0000
n-Heptane	0.0053	0.0049	0.0072
n-Octane	0.0053	0.0017	0.0222
n-Nonane	0.0039	0.0006	0.0198
n-Decane	0.1678	0.0103	0.9113
Cyclohexane	0.0001	0.0001	0.0000
Benzene	0.8044	0.9664	0.0394
Hydrogen	0.0000	0.0000	0.0000
Nitrogen	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
H2O	0.0062	0.0075	0.0000
CO	0.0000	0.0000	0.0000
SULFOLANE	0.0000	0.0000	0.0000
Toluene	0.0000	0.0000	0.0000
o-Xylene	0.0000	0.0000	0.0000
m-Xylene	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000

Figure. (20): T-102 Temperature Profile, Parameters and Compositions: Streams S19.1, S22, and S23: Extraction section PFD stream equivalent 21, 30, and 28

Temperature vs. Tray Position from Top

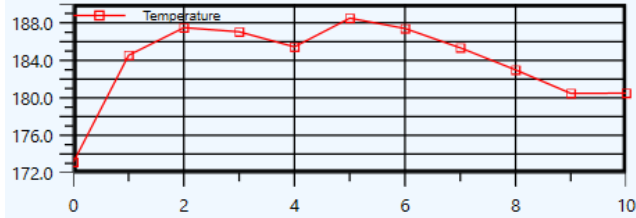


Name	S21 @COL7	S21V @COL7	S21L @COL7
Vapour	0.0275	1.0000	0.0000
Temperature [C]	129.3	123.7	137.8
Pressure [bar]	1.300	1.400	1.300
Molar Flow [kgmole/h]	8427	3400	5027
Mass Flow [kg/h]	4.425e+005	6.495e+004	3.775e+005
Std Ideal Liq Vol Flow [m3/h]	372.6	66.10	306.5
Molar Enthalpy [kcal/kgmole]	-7.633e+004	-5.537e+004	-8.660e+004
Molar Entropy [kJ/kgmole-C]	30.14	131.3	31.50
Heat Flow [kcal/h]	-6.432e+008	-1.882e+008	-4.353e+008

	S21	S21V	S21L
Methane	0.0000	0.0001	0.0000
Ethane	0.0000	0.0001	0.0000
Propane	0.0000	0.0001	0.0000
n-Butane	0.0000	0.0001	0.0000
n-Pentane	0.0001	0.0001	0.0000
n-Hexane	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0001	0.0000
n-Octane	0.0000	0.0001	0.0000
n-Nonane	0.0000	0.0000	0.0000
n-Decane	0.0003	0.0008	0.0000
Cyclohexane	0.0000	0.0000	0.0000
Benzene	0.0067	0.0166	0.0000
Hydrogen	0.0009	0.0022	0.0000
Nitrogen	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
H2O	0.6585	0.9798	0.4412
CO	0.0000	0.0000	0.0000
SULFOLANE	0.3334	0.0000	0.5588
Toluene	0.0000	0.0000	0.0000
o-Xylene	0.0000	0.0000	0.0000
m-Xylene	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000

Figure. (21): T-106 Temperature Profile, Parameters, and Compositions: Streams S21, S21V, and S21L: Extraction section PFD stream equivalent 20, 25, & 24

Temperature vs. Tray Position from Top

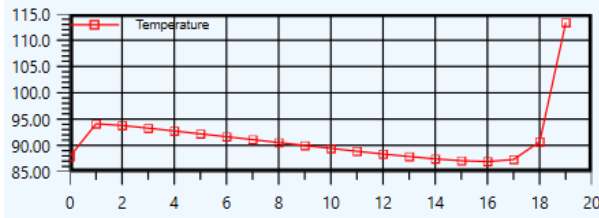


Name	S11.01 @COL8	B/D @COL8	S11V @COL8	S11L @COL8
Vapour	0.0987	0.0000	1.0000	0.0000
Temperature [C]	151.7	50.00	173.1	180.5
Pressure [bar]	1.900	1.200	1.900	1.200
Molar Flow [kgmole/h]	1022	203.0	700.0	525.1
Mass Flow [kg/h]	1.278e+005	2.226e+004	7.531e+004	7.471e+004
Std Ideal Liq Vol Flow [m3/h]	170.4	28.63	97.03	102.0
Molar Enthalpy [kcal/kgmole]	-4.118e+004	-2.886e+004	-1.271e+004	-5.842e+004
Molar Entropy [kJ/kgmole-C]	276.7	71.36	247.6	394.8
Heat Flow [kcal/h]	-4.209e+007	-5.857e+006	-8.898e+006	-3.068e+007

	S11.01	B/D	S11V	S11L
Methane	0.0002	0.0000	0.0003	0.0000
Ethane	0.0004	0.0001	0.0007	0.0000
Propane	0.0004	0.0004	0.0006	0.0000
n-Butane	0.0010	0.0012	0.0018	0.0000
n-Pentane	0.0020	0.0031	0.0038	0.0000
n-Hexane	0.0006	0.0013	0.0013	0.0000
n-Heptane	0.0036	0.0075	0.0075	0.0000
n-Octane	0.0047	0.0080	0.0092	0.0000
n-Nonane	0.0056	0.0063	0.0085	0.0019
n-Decane	0.7337	0.4810	0.4621	0.9981
Cyclohexane	0.0000	0.0001	0.0001	0.0000
Benzene	0.2390	0.4903	0.4912	0.0000
Hydrogen	0.0088	0.0006	0.0130	0.0000
Nitrogen	0.0000	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000	0.0000
H2O	0.0000	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000	0.0000
SULFOLANE	0.0000	0.0000	0.0000	0.0000
Toluene	0.0000	0.0000	0.0000	0.0000
o-Xylene	0.0000	0.0000	0.0000	0.0000
m-Xylene	0.0000	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000	0.0000

Figure. (22): T-107 Temperature Profile, Parameters, Compositions: Streams S11.01, S11V, and S11L: Extraction section PFD stream equivalent 12, 13, and 16

Temperature vs. Tray Position from Top



Name	S22 @COL9	OVP @COL9	OV @COL9	Reformat @COL9
Vapour	1.0000	1.0000	0.0000	0.0000
Temperature [C]	100.4	87.89	87.89	113.4
Pressure [bar]	1.600	1.600	1.600	1.200
Molar Flow [kgmole/h]	295.0	13.00	275.0	7.002
Mass Flow [kg/h]	2.314e+004	901.8	2.144e+004	796.6
Std Ideal Liq Vol Flow [m3/h]	26.48	1.038	24.37	1.066
Molar Enthalpy [kcal/kgmole]	1.922e+004	8715	1.337e+004	-3.776e+004
Molar Entropy [kJ/kgmole-C]	14.08	33.06	-74.52	184.6
Heat Flow [kcal/h]	5.670e+006	1.133e+005	3.678e+006	-2.644e+005

	S22	OVP	OV	Reformat
Methane	0.0000	0.0000	0.0000	0.0000
Ethane	0.0002	0.0043	0.0001	0.0000
Propane	0.0006	0.0076	0.0003	0.0000
n-Butane	0.0021	0.0148	0.0015	0.0000
n-Pentane	0.0043	0.0146	0.0039	0.0000
n-Hexane	0.0013	0.0020	0.0013	0.0000
n-Heptane	0.0049	0.0004	0.0006	0.1805
n-Octane	0.0017	0.0000	0.0000	0.0720
n-Nonane	0.0006	0.0000	0.0000	0.0232
n-Decane	0.0103	0.0000	0.0000	0.4347
Cyclohexane	0.0001	0.0001	0.0001	0.0000
Benzene	0.9664	0.8246	0.9903	0.2896
Hydrogen	0.0000	0.0000	0.0000	0.0000
Nitrogen	0.0000	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000	0.0000
H2O	0.0075	0.1318	0.0018	0.0000

Figure. (23): T-108 Temperature Profile, Parameters and Composition:

Streams S22, OVP, OV, & Reformat: Extraction section PFD stream equivalent 30, 36, 39,& 33

Reformat		
Temperature	87.89	C
Pressure	1.600	bar
Molar Flow	275.0	kgmole/h
Master Comp Mole Frac (Benzene)	0.9903	

Diesel		
Temperature	178.5	C
Pressure	1.200	bar
Molar Flow	829.0	kgmole/h
Master Comp Mole Frac (n-Decane)	0.9776	
Master Comp Mole Frac (n-Nonane)	0.0071	
Master Comp Mole Frac (n-Octane)	0.0054	

Figure. (24): Reformat Final Parameters

Figure. (25): Diesel Product Final Parameters

Name	Hvap3	B/D	Hydrogen
Vapour	0.8903	0.0000	1.0000
Temperature [C]	50.00	50.00	50.00
Pressure [bar]	1.200	1.200	1.200
Molar Flow [kgmole/h]	1850	203.0	1647
Mass Flow [kg/h]	4.774e+004	2.226e+004	2.549e+004
Std Ideal Liq Vol Flow [m3/h]	95.13	28.63	66.50
Molar Enthalpy [kcal/kgmole]	-1105	-2.886e+004	2315
Molar Entropy [kJ/kgmole-C]	135.5	71.36	143.4
Heat Flow [kcal/h]	-2.044e+006	-5.857e+006	3.813e+006

	Hvap3	B/D	Hydrogen
Methane	0.0051	0.0000	0.0057
Ethane	0.0050	0.0001	0.0056
Propane	0.0050	0.0004	0.0056
n-Butane	0.0047	0.0012	0.0051
n-Pentane	0.0041	0.0031	0.0042
n-Hexane	0.0007	0.0013	0.0006
n-Heptane	0.0019	0.0075	0.0012
n-Octane	0.0013	0.0080	0.0004
n-Nonane	0.0008	0.0063	0.0001
n-Decane	0.0558	0.4810	0.0035
Cyclohexane	0.0000	0.0001	0.0000
Benzene	0.1905	0.4903	0.1536
Hydrogen	0.7251	0.0006	0.8144

Figure. (26): Parameters and Composition for V-102:
Streams Hvap3, B/D, and Hydrogen: Extraction section PFD stream equivalent 8, 9, and 10

Name	MS11	MS12	Hvap
Vapour	0.6441	0.0000	1.0000
Temperature [C]	160.0	160.0	160.0
Pressure [bar]	9.200	9.200	9.200
Molar Flow [kgmole/h]	2872	1022	1850
Mass Flow [kg/h]	1.755e+005	1.278e+005	4.774e+004
Std Ideal Liq Vol Flow [m3/h]	265.5	170.4	95.13
Molar Enthalpy [kcal/kgmole]	-1.367e+004	-4.118e+004	1520
Molar Entropy [kJ/kgmole-C]	201.6	293.1	151.1
Heat Flow [kcal/h]	-3.928e+007	-4.209e+007	2.812e+006

	MS11	MS12	Hvap
Methane	0.0034	0.0002	0.0051
Ethane	0.0034	0.0004	0.0050
Propane	0.0034	0.0004	0.0050
n-Butane	0.0034	0.0010	0.0047
n-Pentane	0.0034	0.0020	0.0041
n-Hexane	0.0007	0.0006	0.0007
n-Heptane	0.0025	0.0036	0.0019
n-Octane	0.0025	0.0047	0.0013
n-Nonane	0.0025	0.0056	0.0008
n-Decane	0.2971	0.7337	0.0558
Cyclohexane	0.0000	0.0000	0.0000
Benzene	0.2078	0.2390	0.1905
Hydrogen	0.4702	0.0088	0.7251

Figure. (27): Parameters and Compositions for V-100:
Streams MS11, MS12, Hvap: Extraction section PFD stream equivalent 5, 11, and 6

Name	Alkanes2	Diesel Stream 2	Lights Purge
Vapour	0.1400	0.0000	1.0000
Temperature [C]	182.4	182.4	182.4
Pressure [bar]	1.500	1.500	1.500
Molar Flow [kgmole/h]	280.7	241.4	39.29
Mass Flow [kg/h]	3.917e+004	3.403e+004	5140
Std Ideal Liq Vol Flow [m3/h]	53.28	46.28	6.997
Molar Enthalpy [kcal/kgmole]	-5.685e+004	-5.845e+004	-4.700e+004
Molar Entropy [kJ/kgmole-C]	399.0	392.2	441.3
Heat Flow [kcal/h]	-1.596e+007	-1.411e+007	-1.847e+006
	Alkanes2	Diesel Stream 2	Lights Purge
Methane	0.0000	0.0000	0.0001
Ethane	0.0007	0.0001	0.0046
Propane	0.0001	0.0000	0.0008
n-Butane	0.0009	0.0001	0.0055
n-Pentane	0.0032	0.0009	0.0169
n-Hexane	0.0015	0.0007	0.0066
n-Heptane	0.0109	0.0070	0.0345
n-Octane	0.0156	0.0126	0.0337
n-Nonane	0.0159	0.0149	0.0223
n-Decane	0.9291	0.9504	0.7982
Cyclohexane	0.0000	0.0000	0.0002
Benzene	0.0000	0.0000	0.0000
Hydrogen	0.0053	0.0001	0.0375
Nitrogen	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
H2O	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000
SULFOLANE	0.0167	0.0131	0.0391

Figure (28): Parameters and Compositions for V-101:
Streams Alkanes2, DS2, LP: Extraction section PFD stream equivalent 57, 59, and 58

Name	H2O and Sulf 2	H2O Vap Purge 2	Sulf Ryc	Q X100
Vapour	0.0000	1.0000	0.0000	<empty>
Temperature [C]	137.8	107.1	299.2	<empty>
Pressure [bar]	1.300	1.300	1.300	<empty>
Molar Flow [kgmole/h]	5027	2218	2809	<empty>
Mass Flow [kg/h]	3.775e+005	3.996e+004	3.376e+005	<empty>
Std Ideal Liq Vol Flow [m3/h]	306.5	40.04	266.5	<empty>
Molar Enthalpy [kcal/kgmole]	-8.660e+004	-5.697e+004	-9.278e+004	<empty>
Molar Entropy [kJ/kgmole-C]	31.50	130.9	153.2	<empty>
Heat Flow [kcal/h]	-4.353e+008	-1.264e+008	-2.606e+008	4.833e+007
	H2O and Sulf 2	H2O Vap Purge 2	Sulf Ryc	
H2O	0.4412	1.0000	0.0000	
CO	0.0000	0.0000	0.0000	
SULFOLANE	0.5588	0.0000	1.0000	

Figure. (29): Parameters and Compositions of X-100

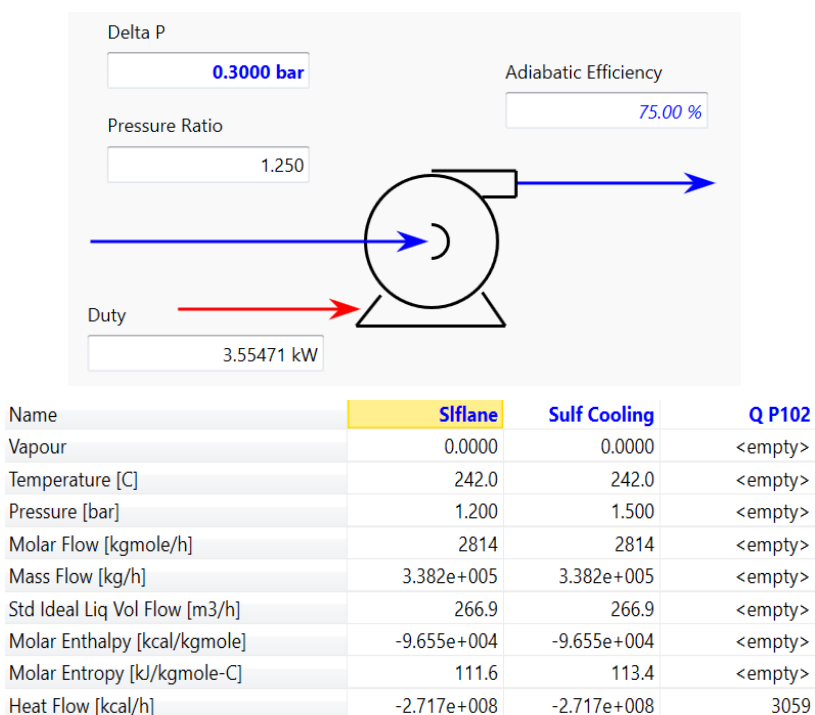


Figure. (30): Parameters and Specifications for P-102:
Streams Siflane and Sulf Cooling: Extraction section PFD stream equivalent 49 and 50

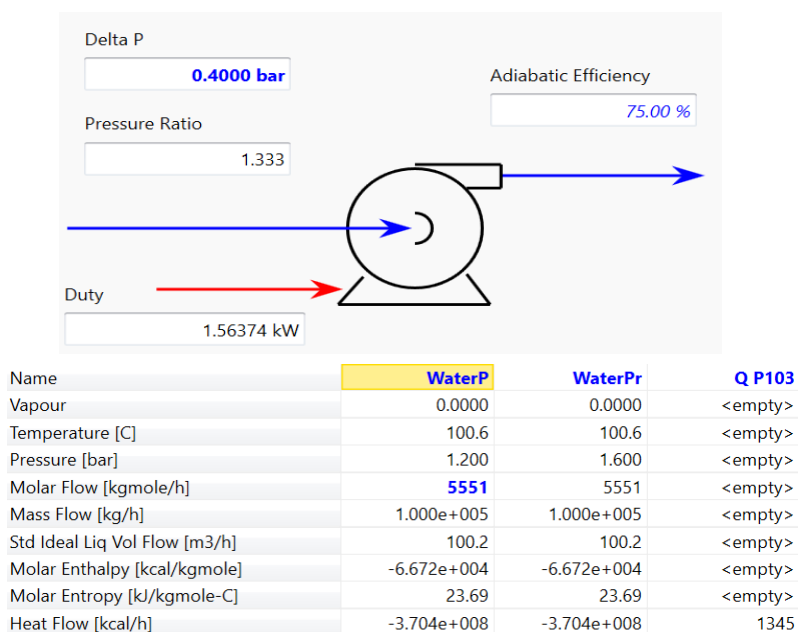
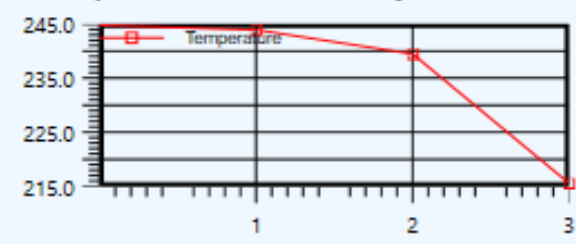


Figure. (31): Parameters and Specifications for P-103:
Streams WaterP and WaterPr: Extraction section PFD stream equivalent 44 and 47

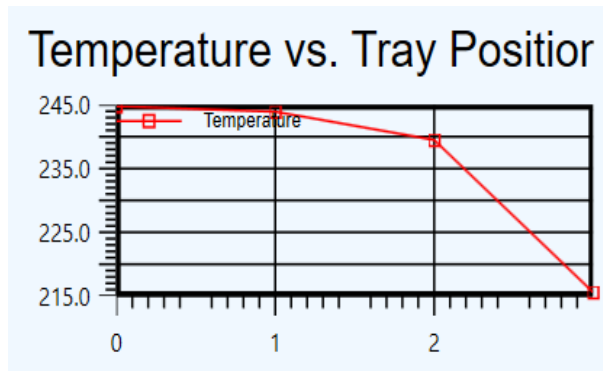
Temperature vs. Tray Position



Name	Sul.2 @COL1	S33R @COL1	S16 @COL1	S17 @COL1
Vapour	0.0000	0.1247	0.0000	0.0000
Temperature [C]	245.0000	110.0000	244.7869	215.5895
Pressure [bar]	1.5000	1.4000	1.5000	1.4000
Molar Flow [kgmole/h]	2814.0893	700.0009	280.6623	3233.4279
Mass Flow [kg/h]	338157.8576	75305.4594	39172.1583	374291.1587
Std Ideal Liq Vol Flow [m3/h]	266.9028	97.0254	53.2775	310.6507
Molar Enthalpy [kcal/kgmole]	-9.636e+004	-2.361e+004	-5.179e+004	-8.448e+004
Molar Entropy [kJ/kgmole-C]	115.7	137.7	452.6	92.93
Heat Flow [kcal/h]	-2.7116e+08	-1.6526e+07	-1.4535e+07	-2.7316e+08

	Sul.2	S33R	S16	S17
Methane	0.0000	0.0003	0.0000	0.0001
Ethane	0.0000	0.0007	0.0007	0.0001
Propane	0.0000	0.0006	0.0001	0.0001
n-Butane	0.0000	0.0018	0.0009	0.0003
n-Pentane	0.0000	0.0038	0.0032	0.0005
n-Hexane	0.0000	0.0013	0.0015	0.0002
n-Heptane	0.0000	0.0075	0.0109	0.0007
n-Octane	0.0000	0.0092	0.0156	0.0006
n-Nonane	0.0000	0.0085	0.0159	0.0005
n-Decane	0.0000	0.4621	0.9291	0.0194
Cyclohexane	0.0000	0.0001	0.0000	0.0000
Benzene	0.0000	0.4912	0.0000	0.1063
Hydrogen	0.0000	0.0130	0.0053	0.0024
Nitrogen	0.0000	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000	0.0000
H2O	0.0000	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000	0.0000
SULFOLANE	1.0000	0.0000	0.0167	0.8689

Figure. (32): Parameters, Composition and Temperature Profile for T-100: Streams Sul.2, S33R, S16, & S17: Extractor section PFD stream equivalent 52, 18, 56, & 19



Name	WaterPr @COL2	S17 @COL2	S19 @COL2	S21 @COL2
Vapour	0.0000	0.0166	0.0000	0.0000
Temperature [C]	100.5754	213.7077	100.6472	180.3863
Pressure [bar]	1.6000	1.4000	1.6000	1.3000
Molar Flow [kgmole/h]	5551.0000	3233.4279	357.4844	8426.9435
Mass Flow [kg/h]	100001.8228	374291.1587	31793.9014	442499.0800
Std Ideal Liq Vol Flow [m3/h]	100.2036	310.6507	38.2621	372.5922
Molar Enthalpy [kcal/kgmole]	-6.672e+004	-8.448e+004	-909.1	-7.633e+004
Molar Entropy [kJ/kgmole-C]	23.69	91.78	4.747	51.93
Heat Flow [kcal/h]	-3.7038e+08	-2.7316e+08	-3.2497e+05	-6.4320e+08

	WaterPr	S17	S19	S21
Methane	0.0000	0.0001	0.0000	0.0000
Ethane	0.0000	0.0001	0.0002	0.0000
Propane	0.0000	0.0001	0.0005	0.0000
n-Butane	0.0000	0.0003	0.0017	0.0000
n-Pentane	0.0000	0.0005	0.0036	0.0001
n-Hexane	0.0000	0.0002	0.0011	0.0000
n-Heptane	0.0000	0.0007	0.0053	0.0000
n-Octane	0.0000	0.0006	0.0053	0.0000
n-Nonane	0.0000	0.0005	0.0039	0.0000
n-Decane	0.0000	0.0194	0.1678	0.0003
Cyclohexane	0.0000	0.0000	0.0001	0.0000
Benzene	0.0000	0.1063	0.8044	0.0067
Hydrogen	0.0000	0.0024	0.0000	0.0009
Nitrogen	0.0000	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000	0.0000
H2O	1.0000	0.0000	0.0062	0.6585
CO	0.0000	0.0000	0.0000	0.0000
SULFOLANE	0.0000	0.8689	0.0000	0.3334

Figure. (33): Parameters, Compositions and Temperature Profile for T-101: Streams WaterPr, S17, S19 and S21: Extraction section PFD stream equivalent 47, 19, 21, & 20

c. Distillation Section Detail

The distillation section had 2 distillation columns, designed to separate and collect Benzene, Toluene and p-Xylene individually. The first of the two collects Benzene from the top stream and sends Toluene and p-Xylene to the second column, where Toluene is collected from the top stream and p-Xylene from the bottom. It was particularly easy to separate Benzene from Toluene due to their relative volatilities (roughly 2.5). It was a bit more difficult to acquire a clean separation of Toluene from p-Xylene due to their relative volatilities, but a method was found in having a lower relative temperature for the top stream (ie. 127.5 °C v/s 148.1°C) and a

somewhat lower pressure in the bottom stream, as well as specifying how much of the p-Xylene would leave the system through the bottom stream. To calculate the composition of the reformat stream used for the distillation section the following equations were used.

$$x_{reformat,benzene} = \frac{\dot{n}_{naphtha} x_{naphtha\ benzene} + (\dot{n}_{reformat} - \dot{n}_{naphtha} x_{naphtha\ benzene}) * 0.11}{\dot{n}_{reformat}}$$

$$x_{reformat,toluene} = \frac{(\dot{n}_{reformat} - \dot{n}_{naphtha} x_{naphtha\ benzene}) * 0.55}{\dot{n}_{reformat}}$$

$$x_{reformat,para-xylene} = \frac{(\dot{n}_{reformat} - \dot{n}_{naphtha} x_{naphtha\ benzene}) * 0.34}{\dot{n}_{reformat}}$$

Figure. (34): Ideal Reformat Composition Equations

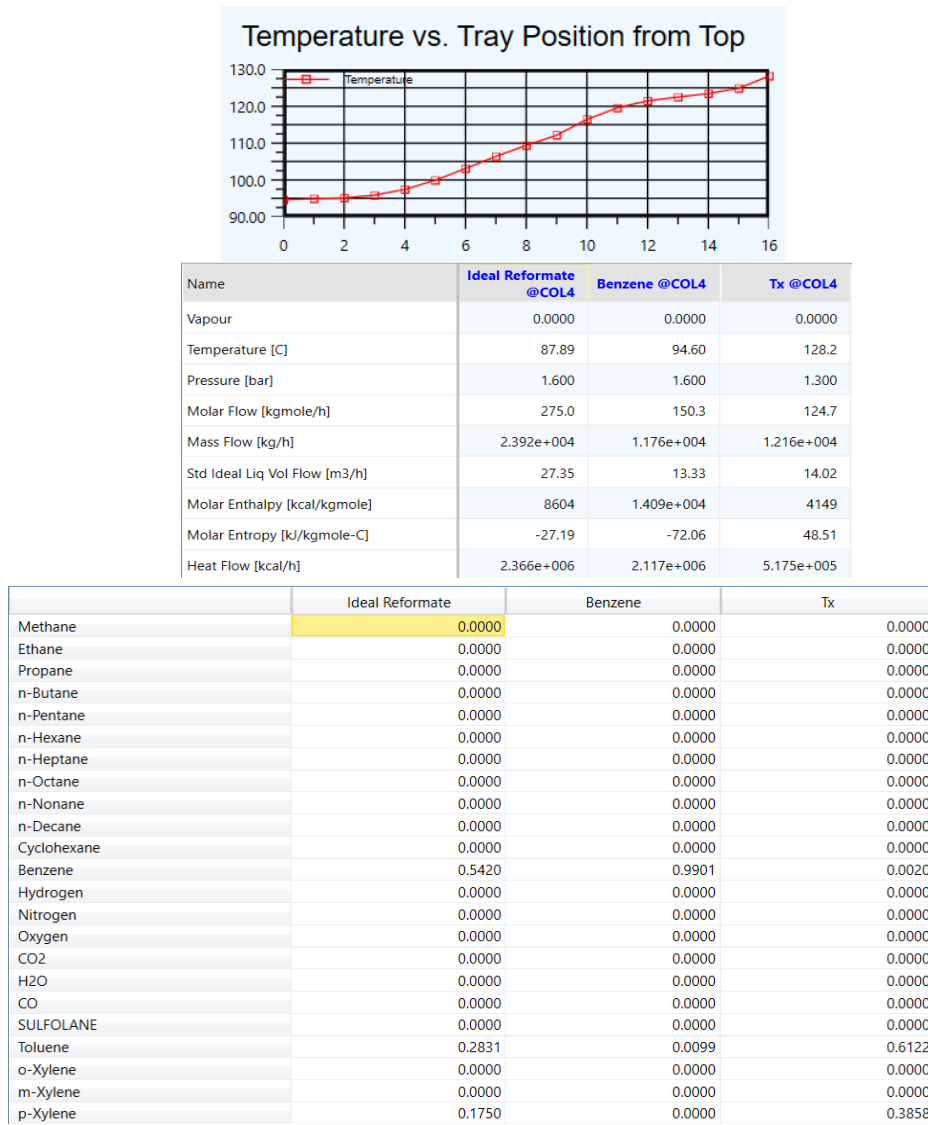
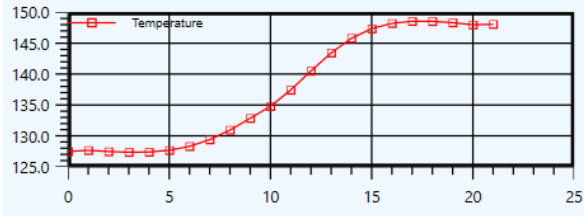


Figure. (35): T-100 Parameters, Composition and Temperature Profile:

Streams Ideal Reformat, Benzene, Tx: Distillation section PFD stream equivalent 1, 6, and 10

Temperature vs. Tray Position from Top



Name	TX @COL5	Toluene @COL5	p-Xylene @COL5
Vapour	0.0000	0.0000	0.0000
Temperature [C]	128.2	127.5	148.1
Pressure [bar]	1.300	1.600	1.300
Molar Flow [kgmole/h]	124.7	76.81	47.91
Mass Flow [kg/h]	1.216e+004	7078	5085
Std Ideal Liq Vol Flow [m3/h]	14.02	8.135	5.883
Molar Enthalpy [kcal/kgmole]	4149	7203	271.9
Molar Entropy [kJ/kgmole-C]	48.51	-12.00	148.7
Heat Flow [kcal/h]	5.175e+005	5.532e+005	1.302e+004

	TX	Toluene	p-Xylene
Methane	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0000
n-Pentane	0.0000	0.0000	0.0000
n-Hexane	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0000	0.0000
n-Octane	0.0000	0.0000	0.0000
n-Nonane	0.0000	0.0000	0.0000
n-Decane	0.0000	0.0000	0.0000
Cyclohexane	0.0000	0.0000	0.0000
Benzene	0.0020	0.0032	0.0000
Hydrogen	0.0000	0.0000	0.0000
Nitrogen	0.0000	0.0000	0.0000
Oxygen	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
H2O	0.0000	0.0000	0.0000
CO	0.0000	0.0000	0.0000
SULFOLANE	0.0000	0.0000	0.0000
Toluene	0.6122	0.9927	0.0020
o-Xylene	0.0000	0.0000	0.0000
m-Xylene	0.0000	0.0000	0.0000
p-Xylene	0.3858	0.0040	0.9980

Figure. (36): T-101 Parameters, Composition and Temperature Profile: Streams TX, Toluene, p-Xylene: Distillation section PFD stream equivalent 10, 15, and 19

Equipment	Base Capital Cost [\$]	Utility Cost [\$/year]	Operator Cost [\$/year]
Distillation Columns			
T-103	960891.97	74515.33	
T-104	641273.19	66354.18	
Costs	1602165.16	140869.51	132635.62
Total	1875670.29		

Table. (34): Distillation Section Column Costs

References

Akhlaq, S.; Khanna, A. Closure Equations in the Estimation of Binary Interaction Parameters. *Korean J. Chem. Eng* 2003, 20 (4), 736–744.

(different Hysys NRTL values for explaining vapor where it shouldn't be in the first lle)

Brondani, L. B.; Flores, G. B.; Soares, R. P. MODELING and SIMULATION of a BENZENE RECOVERY PROCESS by EXTRACTIVE DISTILLATION. *Brazilian Journal of Chemical Engineering* 2015, 32 (1), 283–291. <https://doi.org/10.1590/0104-6632.20150321s00002825>.

Liang, K.; Guo, H.; Pan, S. A Study on Naphtha Catalytic Reforming Reactor Simulation and Analysis. *Journal of Zhejiang University SCIENCE* 2005, 6B (6), 590–596. <https://doi.org/10.1631/jzus.2005.b0590>.

Hassan, A.; Abd, A.; Basil Yousif Khalifa; Fatima Omar Elamin; Nihad Omer Hassan. Evaluation of the Efficiency of the Combustion Furnace of the Delayed Coking Unit by Manipulating the Parameters That Affect the Furnace Efficiency. *American Journal of Quantum Chemistry and Molecular Spectroscopy* 2021, 2 (2), 18. <https://doi.org/10.11648/j.ajqcms.20180202.11>.

Comparative Study of Solvents for the Extraction of Aromatics from Naphtha: Energy Sources: Vol 18, No 1
<https://www.tandfonline.com/doi/pdf/10.1080/00908319608908748?needAccess=true> (accessed Apr 6, 2021).

“Appendix A: Cost Equation and Curve for the HALFCOST Program” *Analysis, Synthesis, and Design of Chemical Processes*, by Richard Turton et al., Prentice Hall, 2018, pp. 1247-1275.

Premkumar, R.; Rangaiah, G. P. Retrofitting Conventional Column Systems to Dividing-Wall Columns. *Chemical Engineering Research and Design* 2009, 87 (1), 47–60. <https://doi.org/10.1016/j.cherd.2008.06.013>.

Gudekar, K. *MODELING, CONTROL, and OPTIMIZATION of FIXED BED REACTORS*; , 2002.