

June 11, 2021

Mr. Abbasi, COO
Kirkuk, Iraq

Dear Mr. Abbasi,

This design team submits the attached proposal entitled *Preliminary Design and Economic Estimate for Kirkuk, Iraq Toppings Refinery Retrofit*.

This proposal investigates strategies for a project that will adhere to Western refining standards; the current product composition contains benzene and does not comply. A fixed bed continuous catalytic reformer is examined as a remedy for its ability to extract benzene from the feedstocks and create BTX. Also discussed in this proposal is the economic feasibility of the project.

Respectfully,
EPC Design Team

AIChE Design Project

Preliminary Design and Economic Estimate for
Kirkuk, Iraq Toppings Refinery Retrofit

Team 9

June 11th, 2021

Executive Summary

The goal of this catalytic reformer retrofit is to manufacture benzene, toluene, and xylene(s) (BTX) as well as diesel and gasoline from the crude feeds K and TQ1 through the same process design. This was achieved with three sections: the reactor section, the extractor section, and the distillation section. The reactor section of this process was modeled after a fixed bed catalytic reformer with a swing reactor for catalyst regeneration. A compressor, 2 stream coolers, 3 fired heaters, 4 reactors, and a vapor separator compose this section. Hazardous components of the naphtha feed were converted to “benzene” through dehydrogenation and cracking reactions. A vapor separator, 8 heat exchangers, a fired heater, 3 pumps, 2 liquid-liquid extractors, and 3 towers make up the extraction section. Here, gasoline and diesel are separated for sale and a reformat stream of 99.7% is sent to the distillation section to be separated into benzene, toluene, para-xylene. A series of 2 distillation columns are employed along with 5 heat exchangers, 3 pumps, and 2 overhead receivers to isolate individual stream components for sale. Feed K had a flowrate of 7,000 BBL/day. Gasoline and diesel products had flowrates of approximately 3,000 and 1,000 BBL/day, respectively. Flowrates of 450, 630, and 450 BBL/day were recorded for benzene, toluene, and para-xylene product streams. Feed K was a priority, but TQ1 was also evaluated and reported in this proposal.

The initial capital investment for this unit was calculated to be \$19.1 Million. In order to operate 30 pieces of equipment, 17 operators are required, and annual operating labor is totaled at \$302,000 annually. Operating labor, as well as annual utility costs of \$142 Million, were included in the yearly incurred manufacturing cost, \$179 Million. These costs are offset by an annual revenue of \$235 Million.

In an effort to determine economic feasibility a cash flow analysis was conducted under both Iraqi and Kurdish tax regimes. The net present value (NPV) under the Iraqi and Kurdish tax regimes was \$110 Million and \$147 Million, respectively. The payback period under Iraqi control is 28 months and 26 months under Kurdish control. The discounted cash flow rate of return (DCFROR) is 57% under Iraqi control, while it is 69% under Kurdish control.

A sensitivity analysis was conducted to study the impact that three different parameters, annual profit, initial investment, and operating cost have on the NPV and DCFROR. Operating cost, annual profit, and initial investment effect these values from greatest to least, respectively.

An inherently safer design (ISD) approach was implemented throughout this design. For example, the system operates at low pressures and temperatures to minimize risk. In addition to ISD techniques process safety management instrumentation and procedures were studied for the major fractionator. A detailed worst-case scenario analysis was conducted, and all hazards were documented in an effort to mitigate risk.

The project has been deemed economically favorable and it is recommended to move forward with a detailed project design with special consideration for FH-103, the reboiler for T-104, as it is a safety concern and will result in the degradation of sulfolane.

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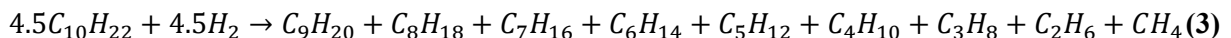
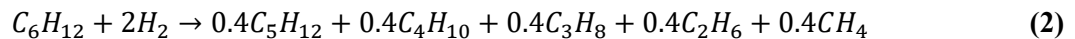
Process Description

The purpose of this design was to process naphthalene from a crude processing unit to produce salable benzene, toluene, and xylenes (BTX), as well as gasoline and diesel. The feed is estimated from two different crude compositions and are referenced as Feed K and Feed TQ1, however the volumetric flowrates of the streams are different. The conditions of each feed stream can be found in Table 1 below.

Table 1: Feed Conditions

		Feed Streams	
		K	TQ1
Pressure [bara]		1.2	1.2
Temperature [°C]		70	70
Naphtha % Volume of Crude		20	28
Naphtha Proxy Components [mol%]	n-decane	59.7	77.8
	cyclohexane	31.3	20.6
	benzene	9	1.6

The simulated design processed both feeds, K and TQ1; both are introduced to the reactor train section of the Naphtha Processing Unit. In this train, which is modeled as a fixed bed continuous catalytic reformer with a swing reactor, there are three heaters and three reactors in series. FH-100 is used as a preheating furnace in order to raise the temperature of the incoming feed stream. Due to the reaction's endothermic nature the fired heaters FH-101 and FH-102 make up for the heat losses in the reactors. The designated reactor feed temperature results in the optimum reactivity and most desired selectivity of each reaction listed. The reactor train in this design modeled three separate fired heaters, however in a detailed design the three fired heaters could be modeled as a single heater with multiple radiant section fireboxes. A list of the reactions present in this process are listed below as equations 1, 2, 3 and 4. The reaction train section of the design is purposed to convert hazardous cyclic and polyaromatic hydrocarbons into benzene, toluene, and xylenes (BTX).¹ All four reactions listed below are taking place in each reactor.



Equation 1 represents the dehydrogenation of cyclohexane to form benzene. Equations 2 and 3 are both cracking reactions. Equation 2 cracks cyclohexane and Equation 3 cracks n-decane to produce shorter chain linear alkanes. Equation 4 produces linear hexane from cyclohexane. Heat integration by E-100 is used to both cool the reaction products and heat the incoming reactant feed. The reaction products are then cooled further by a stream cooler before entering the vapor separator, V-100, which separates hydrogen gas from the reaction products. The top vapor product, hydrogen gas, is recycled to the feed of the reaction section and 10% is purged. Recycled hydrogen is compressed before being re-introduced to the feed.

The bottom product of V-100 is sent to the first stripping column in the extractor section, T-100. This column separates the lighter components, C_1 - C_4 , and sends them out from the top of the stripper for use in the plant. Heavier components are sent on to the first liquid-liquid extractor, T-101. Sulfolane extracts benzene from the incoming stream and the remaining hydrocarbons are sent to the second extractor, T-102, from the top of the T-101. Here, remaining sulfolane in the stream is removed with extraction water. Gasoline and diesel products are produced in the top stream of T-102. The streams exiting the bottom of both extractors are sent to the sulfolane stripper, T-104, where sulfolane is removed from the incoming streams and recycled back into T-101. The top product of T-104, containing mostly benzene, is cooled and sent to the vapor separator, V-101. In this vessel, linear alkanes are separated off as top product, which are sent back into the first extractor, T-101. Liquid bottoms product from V-101, composed of mainly benzene and water, is sent on to the final stripper, T-103. The top stream from this stripper is composed of mostly water, which is split with an 80% purge. The remaining 20% is split again and 70% of this stream is recycled into T-103, while 30% is recycled to T-101. The reformate has a composition of 99.82% “benzene” and is produced from the bottom stream of T-103. The “benzene” is then instantiated, according to the problem statement, into benzene, toluene, and para-xylene. This instantiated stream, the BTX reformate, is sent to the distillation section, where it is processed through two distillation columns in series. In the first distillation column, T-105, salable benzene is separated off the top of the column as product. The bottom stream, composed of para-xylene and toluene, is sent to the second distillation column, T-106. Toluene and para-xylene are separated out as the top stream product and bottom product, respectively.

The optimization of the overall process was considered in each section of the design with safety and economics in mind. Safety considerations were held paramount in the design of each piece of equipment, next to the economic viability of the overall design. For the reactor section, the reactors were designed and scaled to the sizing found in the article titled: “Applying New Kinetic and Deactivation Models in Simulation of a Novel Thermally Coupled Reactor in Continuous Catalytic Regenerative Naphtha Process”.² A reference temperature for the operation of the reactors was sourced from Askari, A., *et. al.* and then varied until greater reaction conversion were obtained for both the K and TQ1 feed streams. A heat integrated preheater was used to increase the temperature of the incoming streams to the reactor train, thereby reducing the usage of fuel gas to heat the feed stream into Reactor 1 by utilizing the high temperature of the outgoing steam from Reactor 3. For the extraction section, each of the strippers were set at a moderate number of stages in order to produce the needed stream compositions, and the pressures of each of the towers were systematically lowered until the given tower could no longer reach the specifications. The number of stages were then reduced to the lowest number of stages possible to meet standards of composition. This allowed the design to operate at the lowest possible operating pressure and temperature to prioritize inherent safety of the design, while also lowering the capital and manufacturing costs. Lowering the pressure of the system as a whole also allowed the design to reduce the number of needed feed pumps and reduce the heat duty for the heat exchangers involved in the process. A similar method was employed for optimizing the distillation section in order to reduce the overall operating temperature and pressure of each of the two distillation columns. This allowed the distillation section to produce the highest purity possible for each of the revenue producing streams, while also prioritizing risk reduction of operation and reducing capital and manufacturing costs for the columns.

Process Flow Diagram

Below are the various process flow diagrams (PFDs), as well as the accompanying stream summary tables. The process flow diagrams are shown in Figures 1-4 and the stream summary tables are shown in Tables 2-6.

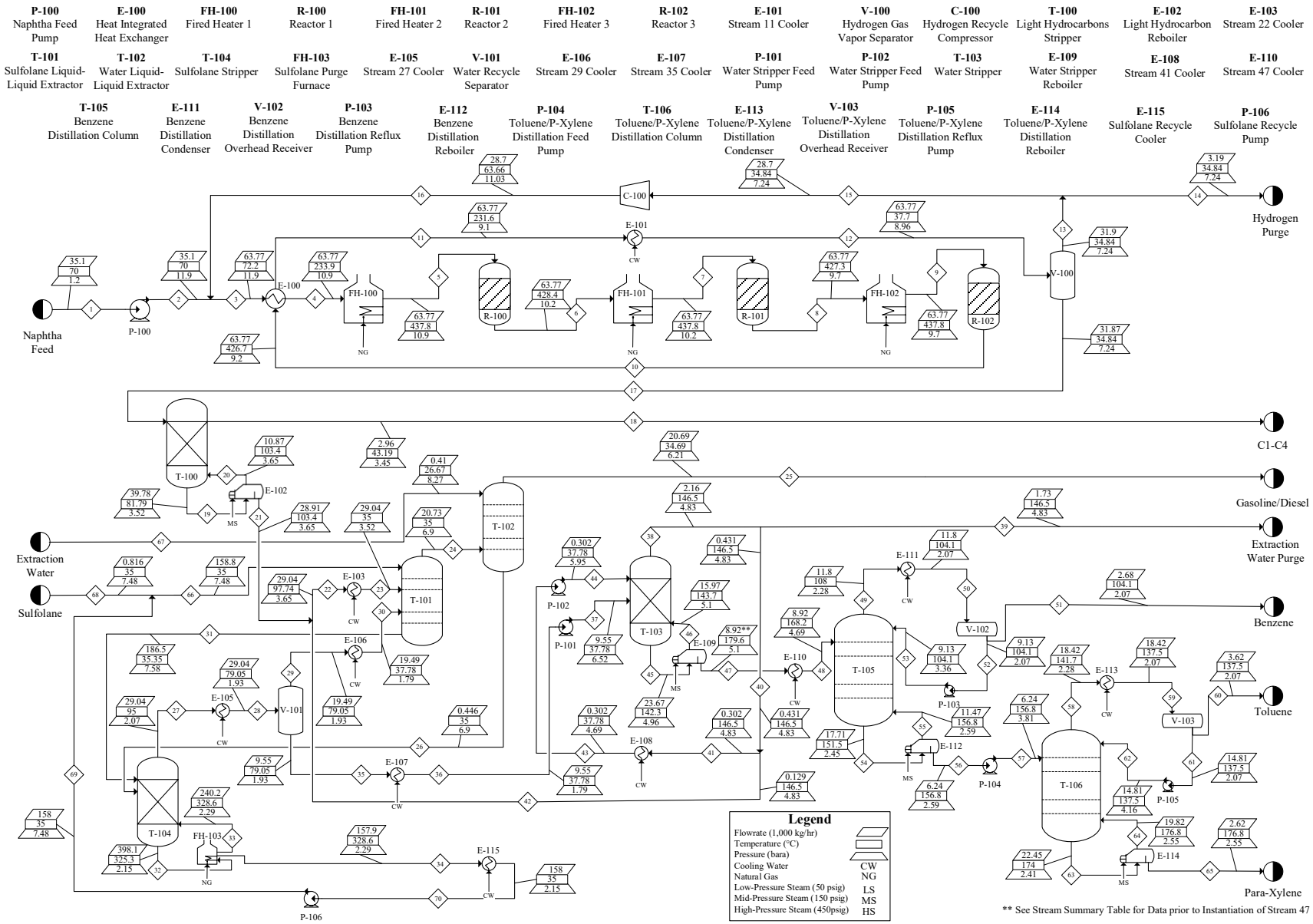


Figure 1: Feed K Overall Process Flow Diagram

P-100 Naphtha Feed Pump
E-100 Heat Integrated Heat Exchanger
FH-100 Fired Heater 1
R-100 Reactor 1
FH-101 Fired Heater 2
R-101 Reactor 2
FH-102 Fired Heater 3
R-102 Reactor 3
E-101 Stream 11 Cooler
V-100 Hydrogen Gas Vapor Separator
C-100 Hydrogen Recycle Compressor

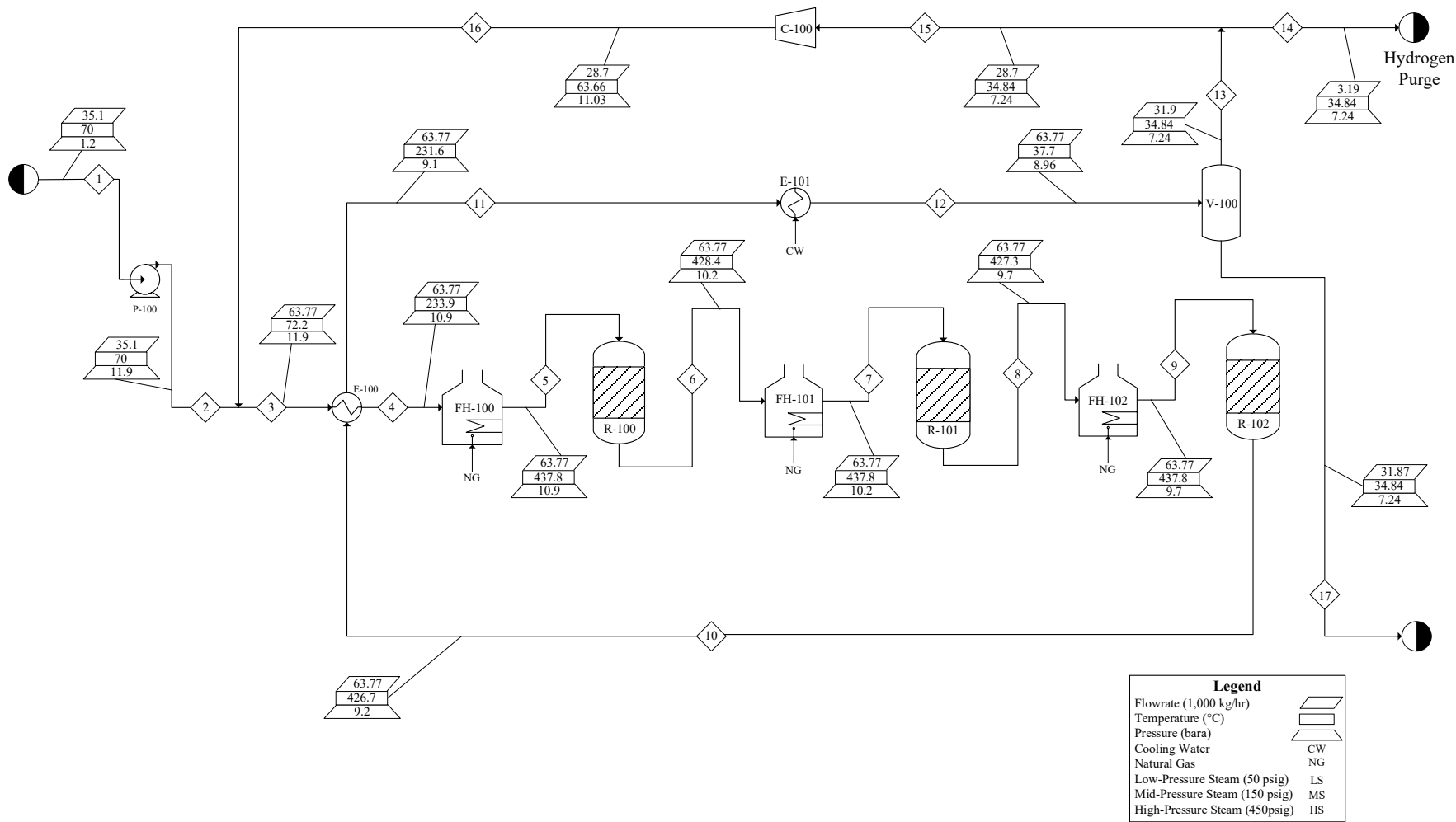


Figure 2: Feed K Reactor Process Flow Diagram

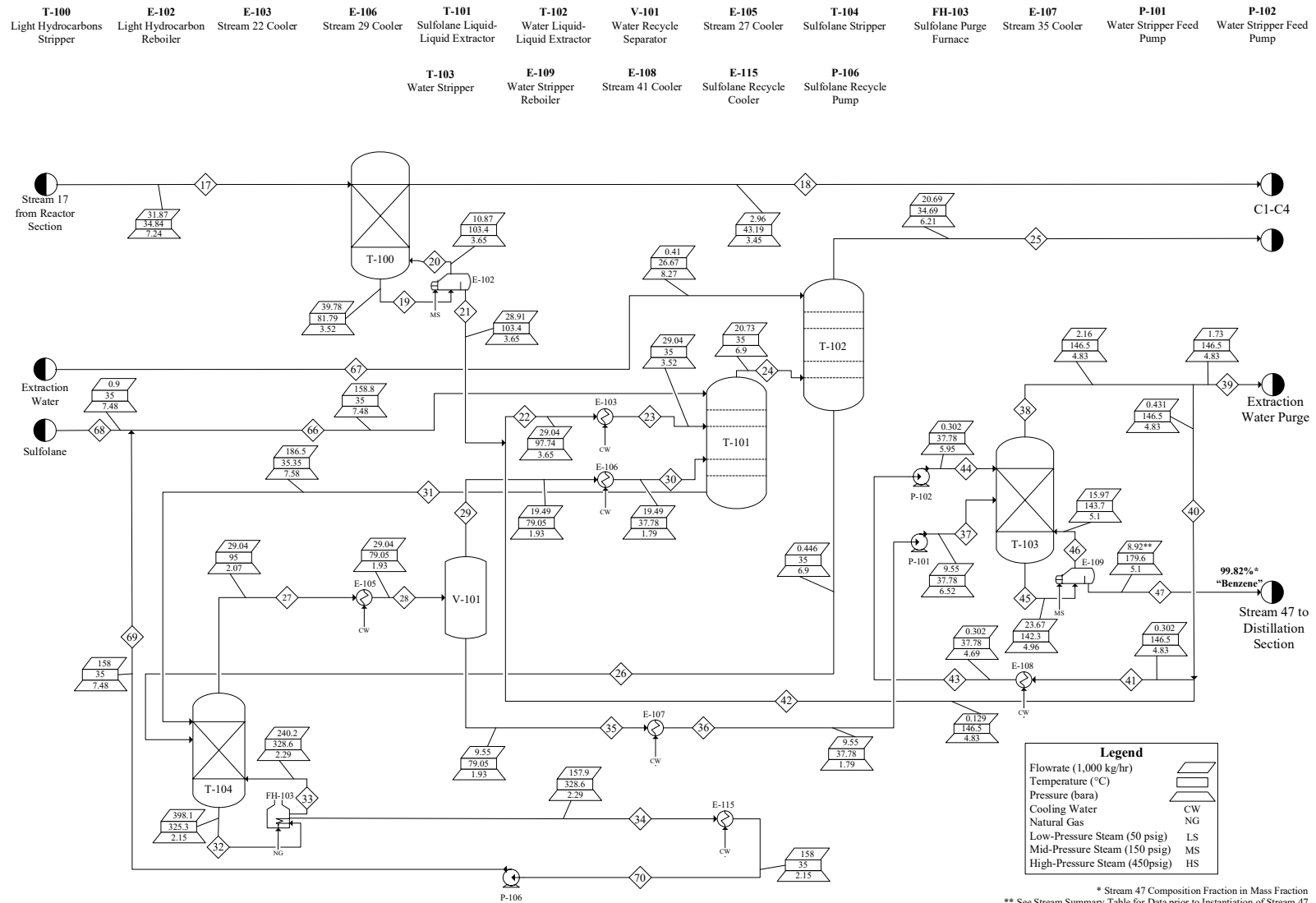
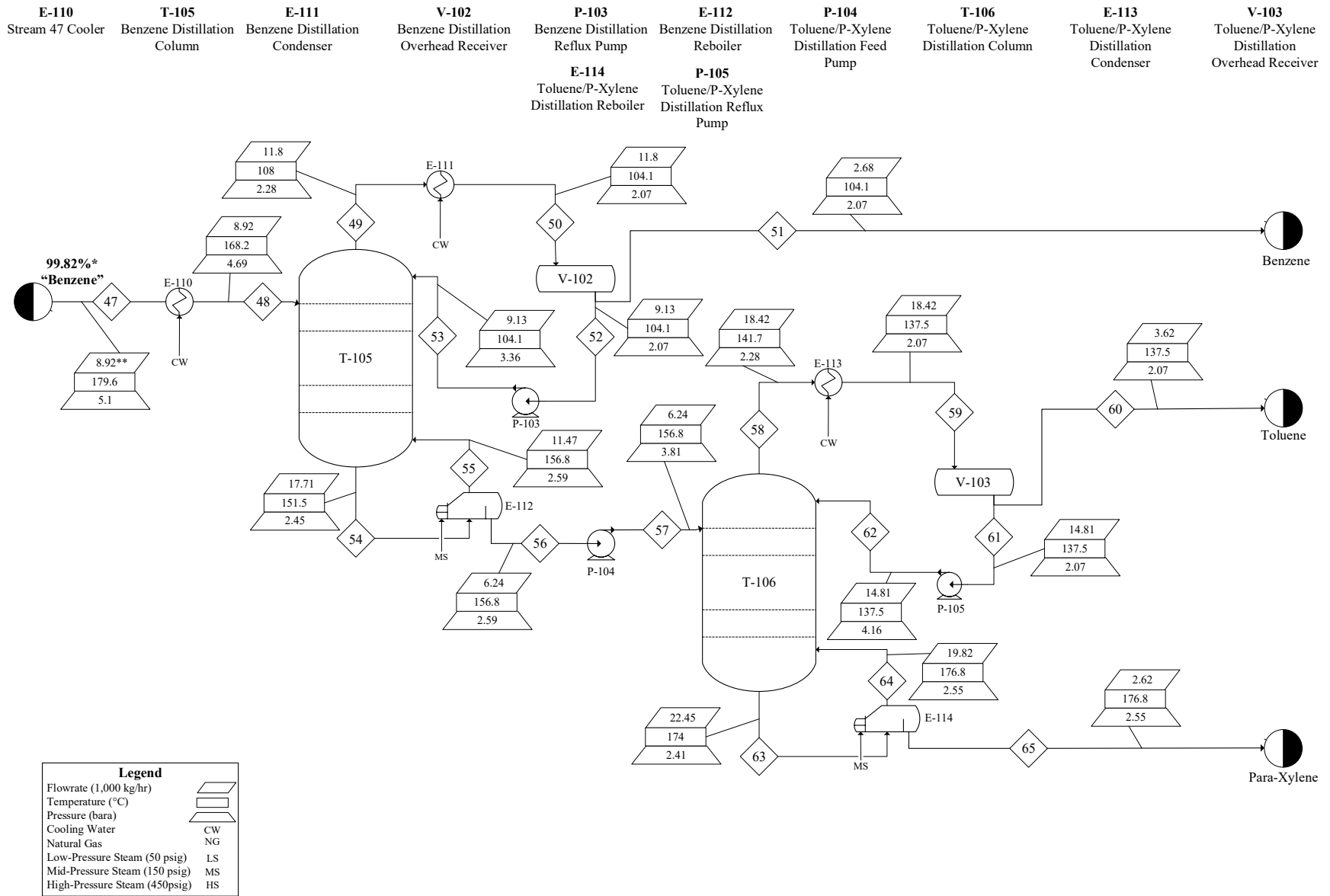


Figure 3: Feed K Extraction Process Flow Diagram



* Stream 47 Composition Fraction in Mass Fraction
 ** See Stream Summary Table for Data prior to Instantiation of Stream 47

Figure 4: Feed K Distillation Process Flow Diagram

Table 2: Stream Summary (Streams 1-15)

Stream Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Stream Descriptions	Naphtha Feed to P-100	P-100 Outlet Stream	Mixture of Stream 2 & Stream 16	E-100 to FH-100	FH-100 to R-100	R-100 to FH-101	FH-101 to R-101	R-101 to FH-102	FH-102 to R-102	R-102 to E-100	E-100 to E-101	E-101 to V-100	Vapor out of V-100	Hydrogen Purge	Vapor to C-100
Vapor Fraction	0.00	0.00	0.758	1	1	1	1	1	1	1	1	1	0.7576	1	1
Temperature [°C]	70.00	70.00	72.22	233.90	437.80	428.40	437.80	427.30	437.80	426.70	231.60	37.78	34.84	34.84	34.84
Pressure [bar]	1.2	11.88	11.88	10.89	10.89	10.20	10.20	9.65	9.65	9.24	9.10	8.96	7.24	7.24	7.24
Molar Flow [kmol/hr]	296.7	296.7	1472	1472	1472	1638	1638	1667	1667	1696	1696	1969	1307	130.7	1176
Mass Flow [kg/hr]	3.51E+04	3.51E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	3.19E+04	3.19E+03	2.87E+04
Molar Enthalpy [kJ/kmol °C]	1.34E+02	1.34E+02	-9.57E+04	-7.11E+04	-4.49E+04	-4.04E+04	-3.92E+04	-3.85E+04	-3.72E+04	-3.66E+04	-5.79E+04	-8.12E+04	-6.79E+04	-6.79E+04	-6.79E+04
Heat Flow [kJ/hr]	-6.28E+07	-6.28E+07	-1.41E+08	-1.41E+08	-6.61E+07	-6.61E+07	-6.42E+07	-6.42E+07	-6.20E+07	-6.20E+07	-9.82E+07	-1.38E+08	-8.87E+07	-8.87E+07	-7.98E+06
Volumetric Flow Rate [m ³ /day]	46.37	46.37	140.70	140.70	140.70	150.50	150.50	156.00	156.00	163.10	163.10	163.10	-	-	-
Mass Density [kg/m ³]	711.70	711.70	21.55	11.19	7.98	6.81	6.72	6.34	6.25	5.97	8.15	16.98	6.90	6.90	6.90
Component Mass Flow [kg/hr]															
n-Decane	25199.7700	25199.7700	25199.7734	25199.7734	25199.7734	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	7814.7200	7814.7200	7814.9110	7814.9110	7814.9110	1.2529	1.2529	1.7101	1.7101	2.3071	2.3071	2.3071	2.3071	0.02155	0.0216
Benzene	2085.5100	2085.5100	2933.1224	2933.1224	2933.1224	7992.0977	7992.0977	8543.6510	8543.6510	9127.6692	9127.6692	9127.6692	939.0626	93.9063	845.1563
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	6163.9277	6163.9277	6163.9277	6988.3860	6988.3860	6955.6476	6955.6476	6920.4191	6920.4191	6920.4191	6853.0716	685.3072	6167.7644
Ethane	0.0000	0.0000	8383.2195	8383.2195	8383.2195	9928.5373	9928.5373	9867.1727	9867.1727	9801.1424	9801.1424	9801.1424	9321.4823	932.1482	8389.3341
Propane	0.0000	0.0000	7429.1767	7429.1767	7429.1767	9695.3590	9695.3590	9605.3707	9605.3707	9508.5383	9508.5383	9508.5383	8267.6455	826.7646	7440.8810
n-Butane	0.0000	0.0000	3520.6054	3520.6054	3520.6054	6507.6469	6507.6469	6389.0306	6389.0306	6261.3962	6261.3962	6261.3962	3926.3312	392.6331	3533.6981
n-Pentane	0.0000	0.0000	1295.0781	1295.0781	1295.0781	5002.9789	5002.9789	4855.7535	4855.7535	4697.3201	4697.3201	4697.3201	1446.6323	144.6632	1301.9691
n-Hexane	0.0000	0.0000	325.3597	325.3597	325.3597	3544.0526	3544.0526	3374.7453	3374.7453	3202.9053	3202.9053	3202.9053	360.7584	36.0758	324.6826
n-Heptane	0.0000	0.0000	129.6863	129.6863	129.6863	4073.4819	4073.4819	4073.4819	4073.4819	4073.4809	4073.4809	4073.4809	144.0390	14.4039	129.6351
n-Octane	0.0000	0.0000	50.8441	50.8441	50.8441	4546.7041	4546.7041	4546.7042	4546.7042	4546.7042	4546.7042	4546.7042	56.5032	5.6503	50.8529
n-Nonane	0.0000	0.0000	22.1806	22.1806	22.1806	5070.1051	5070.1051	5070.1052	5070.1052	5070.1052	5070.1052	5070.1052	24.6436	2.4644	22.1792
Hydrogen	0.0000	0.0000	501.7513	501.7513	501.7513	419.1653	419.1653	486.4031	486.4031	557.7781	557.7781	557.7781	557.2376	55.7238	501.5138
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Sulfolane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	3.51E+04	3.51E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	6.38E+04	3.19E+04	3.19E+03	2.87E+04
Component Mass Fraction															
n-Decane	0.7179	0.7179	0.3952	0.3952	0.3952	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.2226	0.2226	0.1225	0.1225	0.1225	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0594	0.0594	0.0460	0.0460	0.0460	0.1253	0.1253	0.1340	0.1340	0.1431	0.1431	0.1431	0.0294	0.0294	0.0294
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0967	0.0967	0.0967	0.1096	0.1096	0.1091	0.1091	0.1085	0.1085	0.1085	0.2148	0.2148	0.2148
Ethane	0.0000	0.0000	0.1315	0.1315	0.1315	0.1557	0.1557	0.1547	0.1547	0.1537	0.1537	0.1537	0.2922	0.2922	0.2922
Propane	0.0000	0.0000	0.1165	0.1165	0.1165	0.1520	0.1520	0.1506	0.1506	0.1491	0.1491	0.1491	0.2592	0.2592	0.2592
n-Butane	0.0000	0.0000	0.0552	0.0552	0.0552	0.1020	0.1020	0.1002	0.1002	0.0982	0.0982	0.0982	0.1231	0.1231	0.1231
n-Pentane	0.0000	0.0000	0.0203	0.0203	0.0203	0.0785	0.0785	0.0761	0.0761	0.0737	0.0737	0.0737	0.0454	0.0454	0.0454
n-Hexane	0.0000	0.0000	0.0051	0.0051	0.0051	0.0556	0.0556	0.0529	0.0529	0.0502	0.0502	0.0502	0.0113	0.0113	0.0113
n-Heptane	0.0000	0.0000	0.0020	0.0020	0.0020	0.0639	0.0639	0.0639	0.0639	0.0639	0.0639	0.0639	0.0045	0.0045	0.0045
n-Octane	0.0000	0.0000	0.0008	0.0008	0.0008	0.0713	0.0713	0.0713	0.0713	0.0713	0.0713	0.0713	0.0018	0.0018	0.0018
n-Nonane	0.0000	0.0000	0.0003	0.0003	0.0003	0.0795	0.0795	0.0795	0.0795	0.0795	0.0795	0.0795	0.0008	0.0008	0.0008
Hydrogen	0.0000	0.0000	0.0079	0.0079	0.0079	0.0066	0.0066	0.0076	0.0076	0.0087	0.0087	0.0087	0.0175	0.0175	0.0175
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Sulfolane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 3: Stream Summary (Streams 16-30)

Stream Number	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Stream Descriptions	Hydrogen Recycle	Liquid out of V-100	Cl-C4 Purge	T-100 Bottoms to Reboiler	Tops of Reboiler E-102 Return to T-100	Bottoms from Reboiler E-102	Mix of Stream 21 & 42	E-103 to T-101	Light Liquid from T-101	Gasoline & Diesel Product	Heavy Liquid from T-102	Tops from T-104	E-105 to V-102	Vapor from V-102	E-106 to T-101
Vapor Fraction	1	0	1	0	1	0	0.0703	0	0	0	0	1	0.65	1	0
Temperature [°C]	63.66	34.84	43.19	81.79	103.40	103.40	97.74	35.00	35.00	34.69	35.00	95.00	79.05	79.05	37.78
Pressure [bar]	11.03	7.24	3.45	3.52	3.65	3.65	3.65	3.52	6.90	6.21	6.90	2.07	1.93	1.93	1.79
Molar Flow [kmol/hr]	1175	389.5	66.81	476.6	153.9	322.7	328.2	328.2	217	216.80	22.84	508.6	508.6	330.6	330.3
Mass Flow [kg/hr]	2.87E+04	3.19E+04	2.96E+03	3.98E+04	1.09E+04	2.89E+04	2.90E+04	2.90E+04	2.07E+04	2.07E+04	4.46E+02	2.90E+04	2.90E+04	1.95E+04	1.95E+04
Molar Enthalpy [kJ/kmol-°C]	-6.63E+04	-1.26E+05	-9.77E+04	-1.16E+05	-8.41E+04	-1.14E+05	-1.16E+05	-1.30E+05	-2.14E+05	-2.13E+05	-2.87E+05	-4.25E+04	-5.61E+04	-4.17E+04	-7.74E+04
Heat Flow [kJ/hr]	-7.80E+07	-4.90E+07	-6.53E+06	-5.54E+07	-1.29E+07	-3.69E+07	-3.80E+07	-4.28E+07	-4.63E+07	-4.62E+07	-6.55E+06	-2.16E+07	-2.85E+07	-1.38E+07	-2.56E+07
Volumetric Flow Rate [m ³ /day]	-	44.80	5.75	55.52	16.17	39.38	39.51	39.51	30.33	30.30	0.43	35.11	35.11	24.40	24.38
Mass Density [kg/m ³]	9.61	691.80	5.81	648.20	8.24	645.00	122.60	716.10	666.30	665.80	1021.00	3.86	5.78	3.89	771.80
Component Mass Flow [kg/hr]															
n-Decane	0.0000	0.0000	0.0000	0.0000	0.5440	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.1940	2.0916	0.0319	2.6037	2567.3325	2.0597	2.0606	2.0606	1.9906	1.9906	0.0000	0.2196	0.2196	0.1487	0.1496
Benzene	847.6122	8188.6067	141.7219	10614.2173	0.0000	8046.8848	8072.8835	8072.8835	0.9786	0.9785	0.0001	21283.1008	21283.1008	13235.5152	13211.1958
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	6163.9277	67.3475	67.3475	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	8383.2195	479.6601	479.6601	0.0001	0.5009	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	7429.1767	1240.8928	1240.8243	0.5694	3785.4578	0.0685	0.0695	0.0695	0.0321	0.0321	0.0000	1.0745	1.0745	1.0599	1.0371
n-Butane	3520.6054	2335.0650	731.7133	5388.8095	2600.3074	1603.3517	1616.4589	1616.4589	1428.2072	1428.0533	0.1539	4961.3404	4961.3404	4772.0344	4772.9347
n-Pentane	1295.0781	3250.6878	210.1368	5640.8584	926.9559	3040.5510	3041.1196	3041.1196	3036.9733	3036.8901	0.0832	83.8364	83.8364	76.1480	79.6070
n-Hexane	325.3597	2842.1469	52.5941	3716.5087	546.8500	2789.5528	2789.5533	2789.5533	2789.5675	2789.5458	0.0217	0.0334	0.0334	0.0260	0.0259
n-Heptane	129.6863	3929.4430	21.9612	4454.3317	276.8426	3907.4817	3907.4817	3907.4817	3907.4864	3907.4771	0.0093	0.0109	0.0109	0.0063	0.0063
n-Octane	50.8441	4490.2010	8.9840	4758.0596	160.4574	4481.2170	4481.2170	4481.2170	4481.2179	4481.2143	0.0036	0.0039	0.0039	0.0011	0.0011
n-Nonane	22.1806	5045.4616	3.9867	5201.9323	0.0000	5041.4749	5041.4749	5041.4749	5041.4752	5041.4736	0.0016	0.0016	0.0016	0.0003	0.0003
Hydrogen	501.7513	0.5405	0.5405	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	89.7408	89.7408	0.5219	3.7036	405.3982	2961.4411	2691.4411	1404.5030	1403.0293
Sulfolane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	39.9715	0.0000	39.9715	21.8015	21.8015	0.0470	0.0820
Total	2.87E+04	3.19E+04	2.96E+03	3.98E+04	1.09E+04	2.89E+04	2.90E+04	2.90E+04	2.07E+04	2.07E+04	4.46E+02	2.93E+04	2.90E+04	1.95E+04	1.95E+04
Component Mass Fraction															
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.0000	0.0001	0.0000	0.0001	0.2363	0.0001	0.0001	0.0001	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0296	0.2569	0.0479	0.2668	0.0000	0.2783	0.2780	0.2780	0.0000	0.0000	0.0000	0.7261	0.7261	0.6791	0.6786
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
p-Xylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.2150	0.0021	0.0228	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.2924	0.0150	0.1621	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.2591	0.0389	0.4193	0.0000	0.3484	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001
n-Butane	0.1228	0.0733	0.2472	0.1355	0.2393	0.0555	0.0557	0.0557	0.0689	0.0690	0.0003	0.1693	0.1708	0.2449	0.2452
n-Pentane	0.0452	0.1020	0.0710	0.1418	0.0853	0.1052	0.1047	0.1047	0.1465	0.1468	0.0002	0.0029	0.0029	0.0039	0.0041
n-Hexane	0.0113	0.0892	0.0178	0.0934	0.0503	0.0965	0.0961	0.0961	0.1346	0.1348	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0045	0.1233	0.0074	0.1120	0.0255	0.1351	0.1345	0.1345	0.1885	0.1888	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0018	0.1409	0.0030	0.1196	0.0148	0.1550	0.1543	0.1543	0.2162	0.2166	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0008	0.1583	0.0013	0.1308	0.0000	0.1744	0.1736	0.1736	0.2432	0.2437	0.0000	0.0000	0.0000	0.0000	0.0000
Hydrogen	0.0175	0.0000	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0031	0.0031	0.0000	0.0002	0.9097	0.1010	0.0927	0.0721	0.0721
Sulfolane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0019	0.0000	0.0897	0.0007	0.0008	0.0000	0.0000

Table 4: Stream Summary (Streams 31-45)

Stream Number	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	
Stream Descriptions	Bottoms out of T-101	Bottoms from T-104 to FH-103	FH-103 Return to T-104	FH-103 to E-115	Liquid from V-101	E-107 to P-101	P-101 to T-103	Tops from T-103	Extraction Water Purge	T-103 Tops Recycle	Tops of T-103 to E-108	Tops from T-103 to mix with Stream 21	E-108 to P-102	P-102 to T-103	T-103 Bottoms to Reboiler E-109	
Vapor Fraction	0	0	1	0	0	0	0	1	1	1	1	1	0	0	0	
Temperature [°C]	35.35	325.30	328.60	328.60	79.05	37.78	37.78	146.50	146.50	146.50	146.50	146.50	37.78	37.78	142.30	
Pressure [bar]	7.58	2.15	2.29	2.29	1.93	1.79	6.52	4.83	4.83	4.83	4.83	4.83	4.69	5.95	4.96	
Molar Flow [kmol/hr]	1800	3313	1999	1314	178	178	178	92.52	73.97	18.49	12.94	5.548	12.94	12.94	302.9	
Mass Flow [kg/hr]	1.87E+05	3.98E+05	2.40E+05	1.58E+05	9.55E+03	9.55E+03	9.55E+03	2.16E+03	1.73E+03	4.31E+02	3.02E+02	1.29E+02	3.02E+02	3.02E+02	2.37E+04	
Molar Enthalpy [kJ/kmol-°C]	-3.50E+05	-3.81E+05	-3.23E+05	-3.80E+05	-8.28E+04	-8.74E+04	-8.74E+04	-2.12E+05	-2.12E+05	-2.12E+05	-2.12E+05	-2.12E+05	-2.58E+05	-2.58E+05	-2.58E+05	6.64E+04
Heat Flow [kJ/hr]	-6.30E+08	-1.26E+09	-6.46E+08	-4.99E+08	-1.47E+07	-1.56E+07	-1.56E+07	-1.96E+07	-1.57E+07	-3.92E+06	-2.75E+06	-1.18E+06	-3.34E+06	-3.34E+06	-2.01E+07	
Volumetric Flow Rate [m ³ /day]	158.70	315.10	190.10	125.00	10.76	10.76	10.76	2.29	1.83	0.46	0.32	0.14	0.32	0.32	26.80	
Mass Density [kg/m ³]	1158.00	967.90	5.50	964.00	821.90	866.90	866.90	3.23	3.23	3.23	3.23	3.23	899.20	899.20	734.50	
Component Mass Flow [kg/hr]																
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Cyclohexane	0.2196	0.0000	0.0000	0.0000	0.0709	0.0709	0.0709	0.0147	0.0124	0.0031	0.0022	0.0009	0.0022	0.0022	0.0000	
Benzene	21283.1008	0.0000	0.0000	0.0000	8047.5857	8047.5857	8047.5857	433.6013	346.6497	86.6624	60.6637	25.9987	60.6637	60.6637	0.9991	
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
p-Xylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Propane	1.0744	0.0000	0.0000	0.0000	0.0146	0.0146	0.0146	0.0169	0.0131	0.0033	0.0023	0.0010	0.0023	0.0023	0.0000	
n-Butane	4961.1865	0.0000	0.0000	0.0000	189.3060	189.3060	189.3060	219.8896	174.7633	43.6908	30.5836	13.1072	30.5836	30.5836	0.0000	
n-Pentane	83.7533	0.0000	0.0000	0.0000	7.6884	7.6884	7.6884	9.0152	7.5819	1.8955	1.3268	0.5687	1.3268	1.3268	0.0000	
n-Hexane	0.0117	0.0000	0.0000	0.0000	0.0074	0.0074	0.0074	0.0082	0.0066	0.0017	0.0012	0.0005	0.0012	0.0012	0.0000	
n-Heptane	0.0016	0.0000	0.0000	0.0000	0.0046	0.0046	0.0046	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Octane	0.0003	0.0000	0.0000	0.0000	0.0027	0.0027	0.0027	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0013	0.0013	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
H ₂ O	2286.0430	0.0000	0.0000	0.0000	1286.9381	1286.9381	1286.9381	1496.3330	1196.5441	299.1360	209.3952	89.7408	209.3952	209.3952	0.0000	
Sulfolane	157925.2743	398119.6393	240176.1950	157943.4443	21.7544	21.7544	21.7544	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	
Total	1.87E+05	3.98E+05	2.40E+05	1.58E+05	9.55E+03	9.55E+03	9.55E+03	2.16E+03	1.73E+03	4.31E+02	3.02E+02	1.29E+02	3.02E+02	3.02E+02	1.00E+00	
Component Mass Fraction																
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Cyclohexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Benzene	0.1141	0.0000	0.0000	0.0000	0.8424	0.8424	0.8424	0.2008	0.2009	0.2009	0.2009	0.2009	0.2009	0.2009	0.9991	
Toluene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
p-Xylene	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Butane	0.0266	0.0000	0.0000	0.0000	0.0198	0.0198	0.0198	0.0109	0.0103	0.0103	0.0103	0.0103	0.0103	0.0103	0.0000	
n-Pentane	0.0004	0.0000	0.0000	0.0000	0.0008	0.0008	0.0008	0.0042	0.0044	0.0044	0.0044	0.0044	0.0044	0.0044	0.0000	
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	
H ₂ O	0.0123	0.0000	0.0000	0.0000	0.1347	0.1347	0.1347	0.6931	0.6934	0.6934	0.6934	0.6934	0.6934	0.6934	0.0000	
Sulfolane	0.8466	1.0000	1.0000	1.0000	0.0023	0.0023	0.0023	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0009	

Table 5: Stream Summary (Streams 46-60)

Stream Number	46	47	47*	48	49	50	51	52	53	54	55	56	57	58	59	60
Stream Descriptions	Reboiler E-109 Return to T-103	BTX Reformate	Instantiated Reformate	E-110 to T-105	T-105 Tops to Condenser E-111	Condenser E-111 to Overhead Receiver V-102	Benzene Product	Overhead Receiver V-102 Reflux to P-103	P-103 Reflux to T-105	T-105 Bottoms to Reboiler E-112	Reboiler E-112 Return to T-105	Reboiler E-112 to P-104	P-104 to T-106	T-106 Tops to Condenser E-113	Condenser E-113 to Overhead Receiver V-103	Toluene Product
Vapor Fraction	1	0	0.7598	0	1	1	0	0	0	0	1	0	0	1	1	0
Temperature [°C]	143.70	143.70	179.60	168.20	108.00	104.10	104.10	104.10	104.10	151.50	156.80	156.80	156.80	141.70	137.50	137.50
Pressure [bar]	5.10	5.10	5.10	4.69	2.28	2.07	2.07	2.07	3.36	2.45	2.59	2.59	3.81	2.28	2.07	2.07
Molar Flow [kmol/hr]	204.5	98.44	98.25	98.25	151	151	34.24	116.7	116.7	184.5	120.4	64.01	64.01	200.1	200.1	39.28
Mass Flow [kg/hr]	1.60E+04	7.70E+03	8.92E+03	8.92E+03	1.18E+04	1.18E+04	2.68E+03	9.13E+03	9.13E+03	1.77E+04	1.15E+04	6.24E+03	6.24E+03	1.84E+04	1.84E+04	3.62E+03
Molar Enthalpy [kJ/kmol-°C]	9.48E+04	6.61E+04	6.61E+04	4.16E+04	9.07E+04	9.07E+04	6.05E+04	6.05E+04	6.05E+04	2.57E+04	6.02E+04	2.35E+04	2.35E+04	6.48E+04	6.48E+04	3.23E+04
Heat Flow [kJ/hr]	1.94E+07	6.50E+06	6.49E+06	4.09E+06	1.37E+07	1.37E+07	2.07E+06	7.07E+04	7.07E+04	4.74E+06	7.28E+06	1.50E+06	1.50E+06	1.30E+07	1.30E+07	1.27E+06
Volumetric Flow Rate [m ³ /day]	18.09	8.71	10.16	10.16	13.37	13.37	30.32	10.34	10.34	20.32	13.16	7.16	7.16	21.09	21.09	4.14
Mass Density [kg/m ³]	11.50	733.30	16.09	714.90	5.61	5.61	782.50	782.50	782.50	737.10	6.89	731.50	731.50	6.07	6.07	751.80
Component Mass Flow [kg/hr]																
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.1526	0.0584	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	15972.1349	7674.6480	2686.1268	2686.1268	11734.2470	11734.2470	2661.1258	9073.1211	9073.1211	142.4891	117.4882	25.0009	25.0009	127.3960	127.3960	25.0009
Toluene	0.0000	0.0000	3621.1268	3621.1268	69.5575	69.5575	15.7744	53.7830	53.7830	11955.2951	8349.7755	3605.5197	3605.5197	18256.3602	18256.3602	3582.7258
p-Xylene	0.0000	0.0000	2607.8181	2607.8181	0.0000	0.0000	0.0000	0.0000	0.0000	5614.4205	3006.6025	2607.8181	2607.8181	39.3219	39.3219	7.7167
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Pentane	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Hexane	0.0015	0.0004	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0092	0.0045	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0021	0.0027	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0007	0.0013	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Sulfolane	0.3497	21.7544	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Total	1.60E+04	7.70E+03	8.92E+03	8.92E+03	1.18E+04	1.18E+04	2.68E+03	9.13E+03	9.13E+03	1.77E+04	1.15E+04	6.24E+03	6.24E+03	1.84E+04	1.84E+04	3.62E+03
Component Mass Fraction																
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	1.0000	0.9982	0.3013	0.3013	0.9941	0.9941	0.9941	0.9941	0.9941	0.0080	0.0102	0.0040	0.0040	0.0069	0.0069	0.0069
Toluene	0.0000	0.0000	0.4062	0.4062	0.0059	0.0059	0.0059	0.0059	0.0059	0.6750	0.7277	0.5780	0.5780	0.9910	0.9910	0.9910
p-Xylene	0.0000	0.0000	0.2925	0.2925	0.0000	0.0000	0.0000	0.0000	0.0000	0.3170	0.2620	0.4180	0.4180	0.0021	0.0021	0.0021
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Pentane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Sulfolane	0.0000	0.0018	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 6: Stream Summary (Streams 61-70)

Stream Number	61	62	63	64	65	66	67	68	69	70
Stream Descriptions	Overhead Receiver V-103 R reflux to P-105	P-105 Reflux to T-106	T-106 Bottoms to Reboiler E-114	Reboiler E-114 Return to T-106	Para-Xylene Product	Mixture of Stream 68 & 69	Extraction Water Feed	Sulfolane Feed	P-106 to Stream 68 Tee	E-115 to P-106
Vapor Fraction	0	0	0	1	0	0	0	0	0	0
Temperature [°C]	137.50	137.50	174.00	176.80	176.80	35.00	26.67	35.00	35.00	35.00
Pressure [bar]	2.07	4.16	2.41	2.55	2.55	7.48	8.27	7.48	7.48	2.15
Molar Flow [kmol/hr]	160.9	160.9	211.9	187.2	24.74	1359	22.68	1359	1314	1314
Mass Flow [kg/hr]	1.48E+04	1.48E+04	2.25E+04	1.98E+04	2.62E+03	1.59E+05	4.09E+02	8.16E+02	1.58E+05	1.58E+05
Molar Enthalpy [kJ/kmol-°C]	3.23E+04	3.23E+04	7.72E+03	4.22E+04	8.17E+03	-4.47E+05	-2.85E+05	-4.47E+05	-4.53E+05	-4.53E+05
Heat Flow [kJ/hr]	5.19E+06	5.19E+06	1.64E+06	7.90E+06	2.02E+05	-6.08E+08	-6.46E+06	-6.08E+08	-5.95E+08	-5.95E+08
Volumetric Flow Rate [m ³ /day]	16.95	16.95	25.89	22.87	3.03	125.90	0.40	125.90	125.00	125.00
Mass Density [kg/m ³]	751.80	751.80	714.80	7.22	711.70	1245.00	1006.00	1245.00	1247.00	1247.00
Component Mass Flow [kg/hr]										
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	102.3951	102.3951	0.0011	0.0011	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Toluene	14673.6344	14673.6344	339.8913	317.0975	22.7938	0.0000	0.0000	0.0000	0.0000	0.0000
p-Xylene	31.6052	31.6052	22105.2357	19505.1343	2600.1014	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Pentane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	793.7948	408.5798	793.7948	0.0000	0.0000
Sulfolane	0.0000	0.0000	0.0000	0.0000	0.0000	157965.1637	0.0000	21.7200	157943.4443	157943.4443
Total	1.48E+04	1.48E+04	2.24E+04	1.98E+04	2.62E+03	1.59E+05	4.09E+02	8.16E+02	1.58E+05	1.58E+05
Component Mass Fraction										
n-Decane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Cyclohexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Benzene	0.0069	0.0069	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Toluene	0.9910	0.9910	0.0151	0.0160	0.0087	0.0000	0.0000	0.0000	0.0000	0.0000
p-Xylene	0.0021	0.0021	0.9849	0.9840	0.9913	0.0000	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Ethane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Propane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Butane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Pentane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Hexane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Heptane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Octane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
n-Nonane	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Hydrogen	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H ₂ O	0.0000	0.0000	0.0000	0.0000	0.0000	0.0050	1.0000	0.9734	0.0000	0.0000
Sulfolane	0.0000	0.0000	0.0000	0.0000	0.0000	0.9950	0.0000	0.0266	1.0000	1.0000

Economic Analysis and Sensitivities

In an effort to reduce refined fuel import costs in Iraqi Kurdistan, the government is retrofitting existing refineries to compensate for those not adhering to Western safety standards being closed. The proposed design was analyzed under both the Iraqi and Kurdish tax regimes for both feed streams, K and TQ1. A summary of the key economics (net present value [NPV], discounted cash flow rate of return [DCFROR], and payback period) of the cash flow analyses are highlighted in Table 7 below.

Table 7: Cash Flow Highlights

Feed	Tax Regime	NPV	DCFROR	Payback Period [mo.]
K	Iraqi	\$110.1 Million	57%	28
	Kurdish	\$147.2 Million	68%	26
TQ1	Iraqi	\$250.5 Million	96%	21
	Kurdish	\$330.8 Million	114%	19

Bare Module Costs

A breakdown of the equipment costs and annual utility costs can be seen below in Figures 5-8.

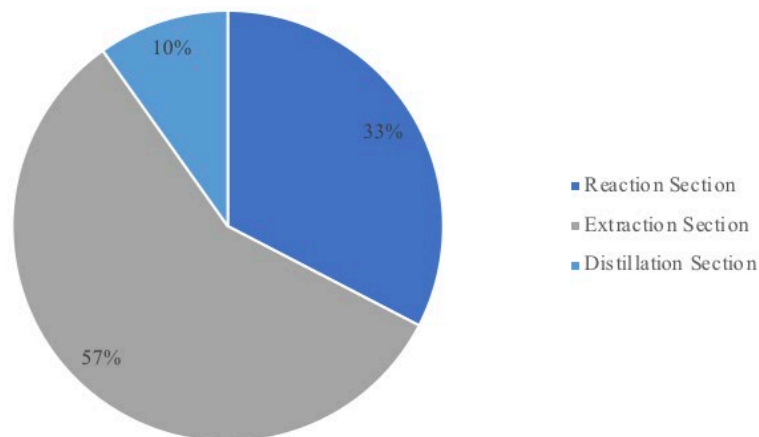


Figure 5: Bare Module Cost Breakdown by Section

Figure 5 illustrates the cost of each individual section, as described by the problem statement. The bare module cost for the entire process was \$16.6 Million. The extraction section came in at \$9.6 Million, or 57% of the bare module cost. The reactor section is \$5.4 Million, or 33% of the cost of

the entire process bare module cost. Lastly, the distillation section is \$1.6 Million, 10% of the total bare module cost, as it was by far the section with the least amount of equipment.

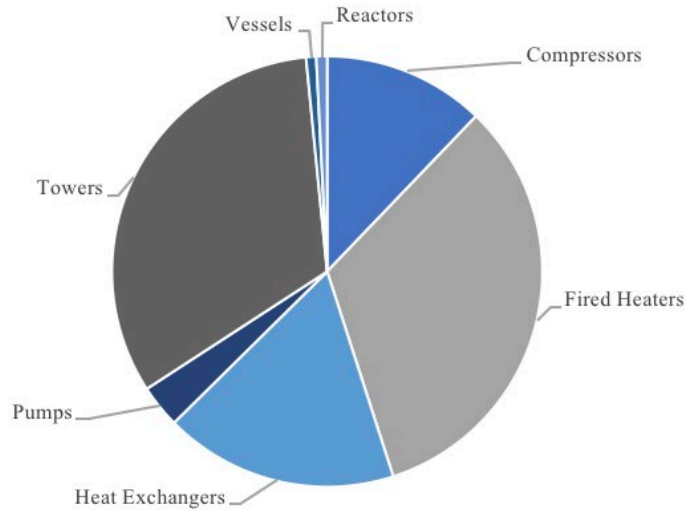


Figure 6: Bare Module Cost by Equipment Type

Bare module costing is broken down into equipment type in Figure 6 above. Towers and fired heaters each cost around 33% of the total bare module cost, \$10.5 Million. The towers are \$5.2 Million, and the fired heaters are \$5.3 Million. The heat exchangers represented 18% of the total bare module cost at \$2.8 Million. The compressor was 12% of the total cost, being \$1.9 Million. Pumps were \$520,000 and represent 3% of the total cost. Lastly, the vessels and reactors were each approximately 1% of the total cost, costing \$120,000 and \$130,000, respectively.

The total bare module cost incurred was \$16.6 Million. This cost only represents the purchase of individual pieces of equipment. The Guthrie Method tacks on an additional 15% to the bare module cost to account for installation of the equipment and provides the total fixed capital cost for the project, \$19.1 Million. The working capital, which covers startup and operation costs before the plant is profitable, is approximately 15% of the fixed capital cost, or \$2.9 Million.⁴

Utility, Operating, and Manufacturing Costs

The utility cost for both feeds was calculated with a 95% service factor to account for maintenance and downtime in the operation. This service factor is standard practice and assumes 346 full days of operation annually.

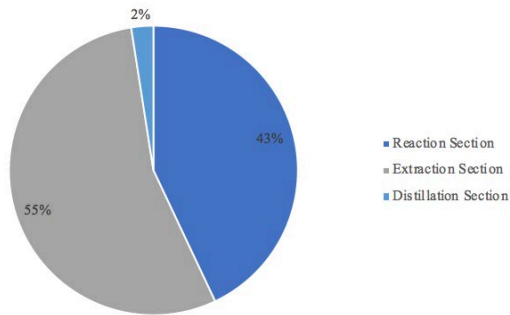


Figure 7: Annual Utility Cost by Section

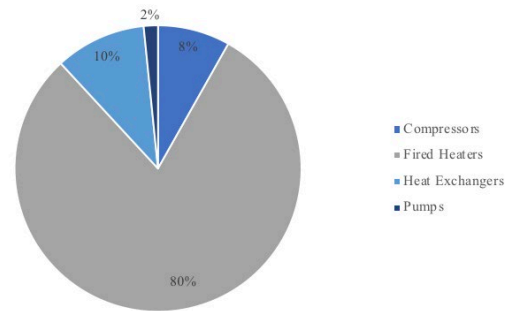


Figure 8: Annual Utility Cost by Equipment Type

Figure 7 above displays the annual utility cost incurred by each section. The reaction section had an annual cost of \$7.7 Million, or 43% of the total annual utility cost. The extraction section, which was 55% of the total annual utility cost was \$9.8 Million. The distillation section represented 2% of the total annual utility cost, coming in at \$444,000 annually. The total annual utility cost to operate the entire process annually is \$18 Million.

According to Figure 8 shown above fired heaters represented the largest expenditure when it comes to the annual utility cost. The fired heaters are 80% of the annual utility cost at \$12 Million. The heat exchangers are 10% of the total annual utility cost at \$1.5 Million. The compressor represents 8% of the annual utility cost at \$1.2 Million. The pumps cost the least to operate costing \$240,000 annually and are 1.6% of the annual utility cost.

The operating labor costs were calculated using the methods shown in Turton, R, *et al.*⁴ The number of operators working were based on the 30 equipment pieces that need to be manned. It should be noted this value only accounts for 3 reactors, as one will always be a not in use. The operators were assumed to have a 40-hour work week making \$8.54/hour.⁵ The wage was a fraction of the United States average in December 2020 because this was the most recent information available. This gives a total annual operating labor cost of \$300,000. It is important to note that this is the only annual cost/revenue that does not apply a 95% service factor to account for paid vacation time. A summarization of the important values is shown below in Table 8.

Table 8: Operating Labor Cost Summary

Sum Number of Equipment	30
Number of Operators per Shift	3.63
Number of Operators	17.00
Annual Work Hours per Operator	2080
Hourly Wage (2020)	\$8.54
Annual Operating Labor Cost	\$302,000

Manufacturing costs are an annual cost that account for utilities and operating labor in addition to raw materials, waste treatment, maintenance, research and development, patents, and much more. Annual manufacturing costs were calculated using Turton, R., *et al.* method and the annual value of manufacturing cost for this design were determined to be \$180 Million and \$235 Million for Feeds K and TQ1, respectively.⁴

Revenue

The revenue for both feeds is summarized in Tables 9 and 10 below. A 95% service factor was applied to account for downtime in the operation.

Table 9: Feed K Revenue

	Benzene	Toluene	Xylene	Gasoline	Diesel
Production (BBL/day)	458.1	627.2	458.1	3181.38	1056.63
Annual Revenue	\$23,283,672.33	\$25,502,762.34	\$18,626,937.87	\$110,494,936	\$57,086,746
Total Annual Revenue K	\$235 Million				

Table 10: Feed TQ1 Revenue

	Benzene	Toluene	Xylene	Gasoline	Diesel
Production (BBL/day)	215.1	806.3	581.3	5478.48	1720.8
Annual Revenue	\$10,932,804.89	\$32,785,199.74	\$23,636,409.04	\$190,277,269	\$92,969,983
Total Annual Revenue TQ1	\$350.6 Million				

From the tables above it can be clearly seen that Feed TQ1 generates more revenue than Feed K. This was to be expected due the greater volume percent of Naphtha for Feed TQ1.

Cash Flow Analysis

Cash flow analyses were completed for both Feed K and TQ1, under both tax regimes. The Iraqi and Kurdish tax rates are 35% and 15%, respectively. The hurdle rate for all analyses is 15%. A 10-year MACRS depreciation rate was used on the capital investment. The cash flow tables indicate that fixed capital costs are incurred in the year 2021; although, startup does not begin until 2023 to allow for plant construction. A ten-year evaluation life was used for all four scenarios of plant operation, under both Iraqi and Kurdish government regulation. The results are given below in Tables 11-14.

The cash flow analysis for inlet Feed K conditions is shown on the next page in Tables 11 and 12. The total fixed capital investment for the unit is \$19 Million. Working capital, incurred in the year 2023, during the startup of the unit, was calculated to be roughly \$3 Million. Manufacturing costs totaled \$180 Million per year, and includes all utility, labor and miscellaneous costs associated with operating on a day-to-day basis. The total revenue generated from the gasoline, diesel, benzene, toluene, and para-xylene product totaled \$235 million on a full-year basis. Under Iraqi control, with the 35% tax rate, the NPV was found to be \$110 Million over the 10-year economic evaluation period. The payback period was found to be 28 months, and the DCFROR was 57%. Under Kurdish control, the NPV was calculated at \$147 Million. The payback period was found to be 26 months, and the DCFROR was 68%. Feed K had a greater NPV and DCFROR under the Kurdish tax regime than the Iraqi. This was expected due to a lower tax deduction of only 15%, under the Kurdish regime, compared to the 35% tax deduction under the Iraqi regime.

Table 11: Cash Flow Analysis of Feed K Under Iraqi Tax Regime

Iraqi Control										
Year	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
End of Year	0	1	2	3	4	5	6	7	8	9
Sales Revenue (Net Revenue)	0	0	117497528	234995055	234995055	234995055	234995055	234995055	234995055	234995055
- Total Manufacturing Costs	0	0	(80645258)	(179290517)	(179290517)	(179290517)	(179290517)	(179290517)	(179290517)	(179290517)
- Depreciation			(2196237)	(3953227)	(3162581)	(2530065)	(2024931)	(1618627)	(1438335)	(1438335)
- Amortization										
- Depletion										
- Writeoff										(3599632)
Taxable Income	0	0	25656032	51751312	52541957	53174473	53679608	54085912	54266003	50666371
- Tax @ 35%	0	0	(8979611)	(18112959)	(18389685)	(18611066)	(18787863)	(18930669)	(18993101)	(17733230)
Net Income	0	0	16676421	33638353	34152272	34563408	34891745	35155843	35272902	32933141
+ Depreciation			2196237	3953227	3162581	2530065	2024931	1618627	1438335	1438335
+ Amortization										
+ Depletion										
+ Writeoff										3599632
- Working Capital				(2864657)						
- Fixed Capital	(19097713)									
Cash Flow	(19097713)	0	16008001	37591579	37314853	37093473	36916676	36774469	36711437	37971309
Discount Factor (P/F _t)	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843
Discounted Cash Flow	(19097713)	0	12104349	24717074	21334839	18442012	15960098	13824835	12001034	10793816
NPV (Year 0) @ hurdle rate =	\$110 Million									
Payback Period [months] =	28									
DCFRROR =	57%									

Table 12: Cash Flow Analysis of Feed K Under Kurdish Tax Regime

Kurdish Control										
Year	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
End of Year	0	1	2	3	4	5	6	7	8	9
Sales Revenue (Net Revenue)	0	0	117497528	234995055	234995055	234995055	234995055	234995055	234995055	234995055
- Total Manufacturing Costs	0	0	(80645258)	(179290517)	(179290517)	(179290517)	(179290517)	(179290517)	(179290517)	(179290517)
- Depreciation			(2196237)	(3953227)	(3162581)	(2530065)	(2024931)	(1618627)	(1438335)	(1438335)
- Amortization										
- Depletion										
- Writeoff										(3599632)
Taxable Income	0	0	25656032	51751312	52541957	53174473	53679608	54085912	54266003	50666371
- Tax @ 15%	0	0	(3848405)	(7762697)	(7881294)	(7976171)	(8051941)	(8112887)	(8139900)	(7599956)
Net Income	0	0	21807627	43988615	44660663	45198302	45627667	45973025	46126103	43066415
+ Depreciation			2196237	3953227	3162581	2530065	2024931	1618627	1438335	1438335
+ Amortization										
+ Depletion										
+ Writeoff										3599632
- Working Capital				(2864657)						
- Fixed Capital	(19097713)									
Cash Flow	(19097713)	0	21139207	47941842	47823245	47728367	47652597	47591652	47564638	48104583
Discount Factor (P/F _t)	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843
Discounted Cash Flow	(19097713)	0	15984278	31522539	27343095	23729434	20601533	17891466	15548964	13674325
NPV (Year 0) @ hurdle rate =	\$147 Million									
Payback Period [months] =	26									
DCFRROR =	68%									

Table 13: Cash Flow Analysis of Feed TQ1 Under Iraqi Tax Regime

Iraqi Control										
Year	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
End of Year	0	1	2	3	4	5	6	7	8	9
Sales Revenue (Net Revenue)	0	0	175300833	350601666	350601666	350601666	350601666	350601666	350601666	350601666
- Total Manufacturing Costs	0	0	(116888317)	(233616634)	(233616634)	(233616634)	(233616634)	(233616634)	(233616634)	(233616634)
- Depreciation			(2196237)	(3953227)	(3162581)	(2530065)	(2024931)	(1618627)	(1438535)	(1438535)
- Amortization										
- Depletion										
- Writeoff										(3599632)
Taxable Income	0	0	56296279	113031805	113822450	114454966	114960101	115366405	115546496	111946864
- Tax @ 35%	0	0	(19703698)	(39561132)	(39837858)	(40059238)	(40236035)	(40378242)	(40441274)	(39181402)
Net Income	0	0	36592581	73470673	73984593	74395728	74724066	74988163	75105222	72765461
+ Depreciation			2196237	3953227	3162581	2530065	2024931	1618627	1438535	1438535
+ Amortization										
+ Depletion										
+ Writeoff										3599632
- Working Capital			(2864657)							
- Fixed Capital	(19097713)									
Cash Flow	(19097713)	0	35924161	77423900	77147174	76925793	76748996	76606790	76543758	77803629
Discount Factor (P/F _{t,n})	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843
Discounted Cash Flow	(19097713)	0	27163827	50907471	44109147	38245715	33180709	28799330	25022290	22116647
NPV (Year 0) @ hurdle rate =	\$250 Million									
Payback Period [months]=	21									
DCFRROR =	96%									

Table 14: Cash Flow Analysis of Feed TQ1 Under Kurdish Tax Regime

Kurdish Control										
Year	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030
End of Year	0	1	2	3	4	5	6	7	8	9
Sales Revenue (Net Revenue)	0	0	175300833	350601666	350601666	350601666	350601666	350601666	350601666	350601666
- Total Manufacturing Costs	0	0	(116888317)	(233616634)	(233616634)	(233616634)	(233616634)	(233616634)	(233616634)	(233616634)
- Depreciation			(2196237)	(3953227)	(3162581)	(2530065)	(2024931)	(1618627)	(1438535)	(1438535)
- Amortization										
- Depletion										
- Writeoff										(3599632)
Taxable Income	0	0	56296279	113031805	113822450	114454966	114960101	115366405	115546496	111946864
- Tax @ 15%	0	0	(8444442)	(16954771)	(17073368)	(17168245)	(17244015)	(17304961)	(17331974)	(16792030)
Net Income	0	0	47851837	96077034	96749083	97286721	97716086	98061444	98214522	95154834
+ Depreciation			2196237	3953227	3162581	2530065	2024931	1618627	1438535	1438535
+ Amortization										
+ Depletion										
+ Writeoff										3599632
- Working Capital			(2864657)							
- Fixed Capital	(19097713)									
Cash Flow	(19097713)	0	47183417	100030261	99911664	99816786	99741016	99680071	99633057	100193002
Discount Factor (P/F _{t,n})	1.0000	0.8696	0.7561	0.6575	0.5718	0.4972	0.4323	0.3759	0.3269	0.2843
Discounted Cash Flow	(19097713)	0	35677442	65771520	57124818	49626584	43120794	37473431	32576761	28481104
NPV (Year 0) @ hurdle rate =	\$330 Million									
Payback Period [months]=	19									
DCFRROR =	114%									

Similar trends between tax regimes for Iraq and Kurdistan were observed for the Feed TQ1 cash flow analyses, where the Kurdish tax regime resulted in greater NPV and DCFROR, as well as a shorter payback period. The cash flow analyses for inlet stream TQ1 are shown on the previous page in Tables 13 and 14. The fixed capital investment and working capital for the unit utilizing Feed TQ1 is equal to that of Feed K: \$19 Million and \$3 Million, respectively. Manufacturing costs for operation using TQ1 is \$234 Million during a full year of operation. This is due to the increased feed flow from TQ1. Total revenue generated from the production streams using TQ1 is \$350 million. Using the Iraqi tax rate of 35%, the NPV is \$250 million, the payback period is 21 months, and the DCFROR is 96%. Under the Kurdish tax rate of 15%, the NPV is \$330 million, the payback period is 19 months, and the DCFROR is 114%.

Comparing the cash flow analyses between Feed K and TQ1 shows that both feeds are profitable, although TQ1 is more so. Subsequently, TQ1 has a higher NPV and DCFROR, as well as a lower payback period. This is to be expected, because capital cost is the same between the two, while the annual profit for TQ1 is greater. The annual manufacturing costs for TQ1 are \$50 Million higher than that of feed K. However, TQ1 revenue exceeds that of K by more than \$100 Million, resulting in a higher profit margin for TQ1.

Sensitivity Analysis

Figures 9-12 below are the tornado charts for the net present values of Feed K and TQ1 under both Iraqi and Kurdish tax regimes.

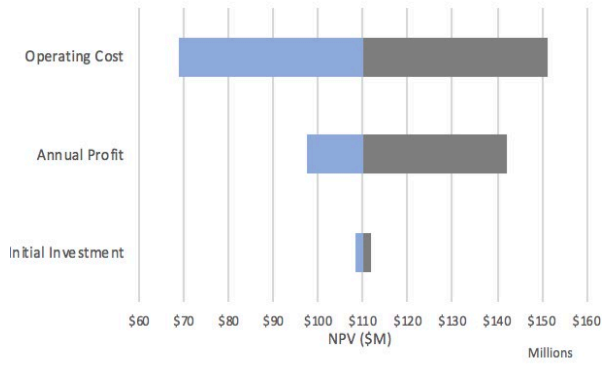


Figure 9: NPV Tornado Chart for Feed K & Iraqi Tax Regime

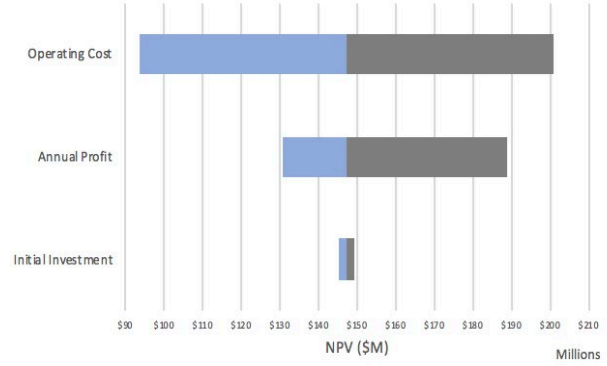


Figure 10: NPV Tornado Chart for Feed K & Kurdish Tax Regime

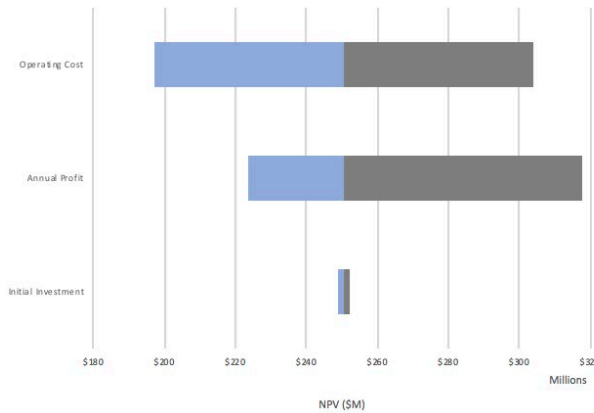


Figure 11: NPV Tornado Chart for Feed TQ1 & Iraqi Tax Regime

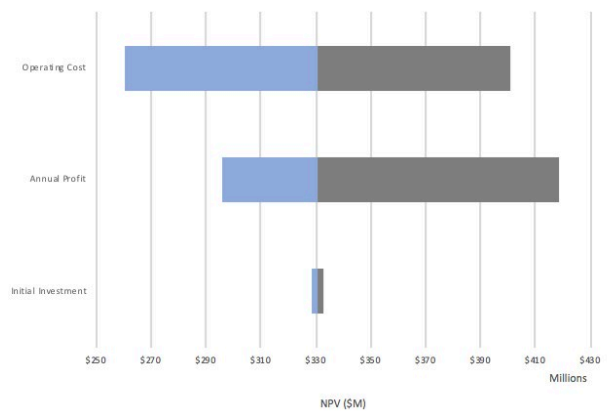


Figure 12: NPV Tornado Chart for Feed TQ1 & Kurdish Tax Regime

The tornado charts for the NPV show how different variables affect the economics of this design. The three variables considered were: operating cost, annual profit, and the initial investment, or the fixed capital investment. The most significant of the three variables considered was the operating cost, which was varied by +/- 10%. This parameter is most significant because of the effect it has on the profitability in each year of the analysis. Under both tax regimes the change in operating cost cause the NPV to vary by approximately +/- 35% for Feed K, and +/- 20% for Feed

TQ1. The second most significant parameter was the annual profit, as this was varied by +25% and -10%. The NPV changed by roughly the same percentage. The initial investment had the smallest impact on the NPV of the unit. Initial investment was changed by +/- 10%. The NPV varied by nearly +/- 1% from the base case for all for analyses. This variable had the least impact on NPV since the size of the initial investment was significantly smaller than the amount of positive cash flow on a full year of operation.

Figures 13-16 below are the tornado charts for the DCFROR values of feeds K and TQ1 under both Iraqi and Kurdish tax regimes.

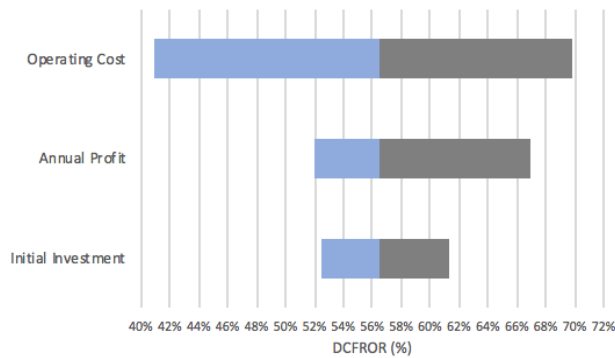


Figure 13: DCFROR Tornado Chart for Feed K & Iraqi Tax Regime

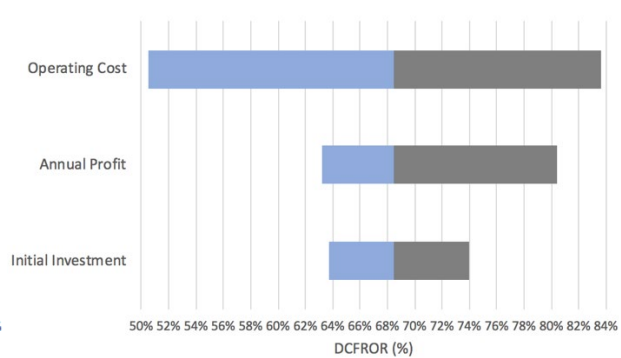


Figure 14: DCFROR Tornado Chart for Feed K & Kurdish Tax Regime

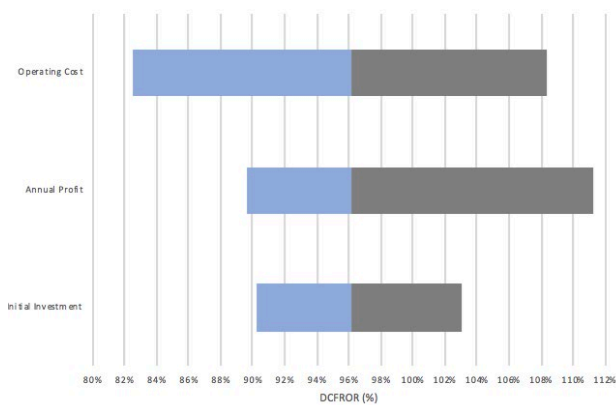


Figure 15: DCFROR Tornado Chart for Feed TQ1 & Iraqi Tax Regime

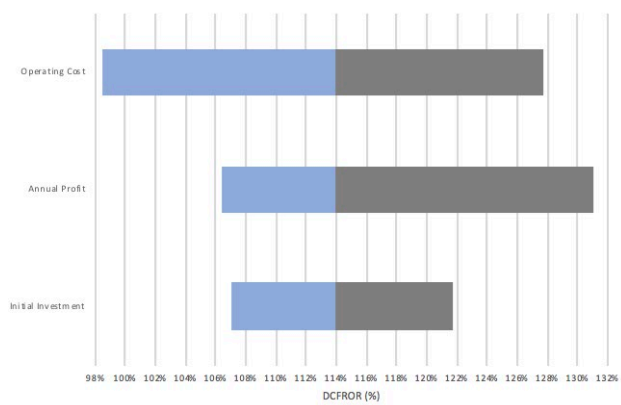


Figure 16: DCFROR Tornado Chart for Feed TQ1 & Kurdish Tax Regime

A sensitivity analysis was also conducted for the DCFROR of Feed K and TQ1 under both tax regimes. The three parameters and their variance were the same as those chosen for the NPV. The

DCFRROR followed the same trends seen from the NPV analysis. Operating cost had the biggest impact, followed by the annual profit and the initial invest had the smallest impact. The operating cost was varied by +/- 10%. Feed K under Iraqi and Kurdish tax regimes experienced approximately -28% to 23% change; whereas, Feed TQ1 under both regimes was -14% to 12%. The operating cost changes the rate at which the profit pays the debt by decreasing the positive cash flow on an annual basis, which is why this variable holds so much sway on DCFRROR. The annual profit, varied by +25% and -10%, Feed K experienced a -8% to 18% variance. DCFRROR is based on the yearly positive income and the rate at which the investment is paid off, not the total profit as a whole over the economic evaluation life. Given the magnitude of the annual profit versus other parameters, it is understandable that this variable has a fairly large effect on the overall DCFRROR. The initial investment has the smallest impact on the DCFRROR. When initial investment was varied by +/- 10% Feed K experienced a -7% to 8% variance and Feed TQ1 experienced a -6% to 7% variance from the base DCFRROR. This is because the level of annual profit is much higher than the initial investment. With a low payback period and a high annual profit, the DCFRROR is only slightly affected by the increase in the fixed capital investment.

Process Safety

Inherent Safety Evaluation

Safety was an integral part of the process design. First and foremost, inherent safety techniques were employed to mitigate hazards and risks as much as possible. Inherently safer design strategies are minimization, moderation, substitution, and simplification. All of these inherently safer design methods were utilized in this design. Each strategy will be explained in depth as towards how it was implemented during the design process, as well as additional safety concerns to be further investigated or avoided in a detailed design.

The minimization technique was employed in this design by use of a heat-integrated heat exchanger, E-100. Heat from the products leaving the reactors is used to heat the incoming feed stream to Reactor 1. This reduces the required amount of fuel gas by FH-100 to heat the reactor section feed stream. Minimization can also be implemented in the detailed design by use of a divided wall column, where two distillation columns of the process could be consolidated into one piece of equipment. Not only would a divided wall column save on energy consumption, but it

would also reduce capital costs. Minimization of this form reduces the total number of columns in the process and, therefore, consequence of incidents.

Moderation methods create a safer design by reducing hazardous materials or conditions and were considered when designing the operating conditions of the process. The entire system operates at less severe process conditions. A low-pressure system reduces the probability and consequence of an incident, as well as capital cost and the cost of operation. Some of the columns in this design did not require feed pumps, as the pressure of the feed exceeded the required operating pressure within the column. This instance also exhibits use of simplification as a safety method implemented by the design, discussed later. Table 15 summarizes conditions of the columns in the process.

Table 15: Column Design Summary

Column Tag	Feed Pump?	Operating Pressure [bara]	Operating Temperature [°C]
T-100	No	3.65	81.79
T-103	Yes	5.1	143.7
T-104	No	2.29	328.6
T-105	No	2.59	156.8
T-106	Yes	2.55	176.8

Although the process was designed with relatively low temperatures, there are a few notable exceptions to address. In order for the reactions to take place the reaction section is operating above 400°C. It is important to note that considering the fire risk associated with the components in the reactor train, the temperatures are below the auto-ignition value for any single component. Although high temperatures are necessary, it poses a safety hazard that must be considered in future detailed design. Extrinsic, as well as procedural safety techniques will need to be employed for optimally safe operation.

Simplification of a process is defined by minimizing complexity of design, such as reducing the amount of equipment. For instance, the low-pressure conditions of the process allowed for simplification by eliminating the need for feed pumps for the columns. The removal of 3 unnecessary feed pumps decreases risk in the process. Mechanical failure is the most common cause for losses, therefore eliminating unnecessary equipment removes the risk associated with operating the equipment all together. The heat integration of E-100 also demonstrates the use of

simplification as a means to reduce process hazards by eliminating the need for additional fuel gas or steam.

Another technique that was used throughout the design process was substitution. Replacement of hazardous process materials, reaction chemistry, and construction material can reduce risk of the design. For instance, heating and cooling media can vary in their toxicity and flammability. Cooling water was chosen as the utility fluid for all stream coolers and condensers. This is a cheaper utility option, as well as less hazardous and non-flammable, when compared to some other refrigerants. The utility fluid chosen for all reboilers was medium-pressure steam, 150 psig. Most of the reboilers in the process could not operate on a low-pressure steam, 50 psig. Medium-pressure steam proved to be the most cost effective for the reboilers, as well as fulfill the energy requirements to achieve the level of heating required. This option for steam was chosen over high-pressure steam, provided at 450 psig, because it is of an inherently safer design with a lower supply pressure. Low-carbon carbon steel, which consists of $>0.3\%$.⁶ Carbon steel was found to be the most used material option in the process design. This material of construction was chosen for many reasons; Low-carbon carbon steel is the cheapest carbon steel option and it is the most ductile. Ductility is directly correlated with material inherent safety. A high ductility material allows for malleability under pressure, whereas a brittle material would break instead. Other than the choice of carbon steel some pieces of equipment were decided to be constructed out of Nickel Alloy. This option was pursued when sulfolane was present in the stream to protect from equipment corrosion, but it also is more ductile than the carbon steel option proving to lower risk even more. These inherent safety techniques were implemented throughout the design process to minimize risk as much as possible at this stage. Additional layers of protection will be analyzed throughout project life.

Using the methods of an inherently safer design mitigates many potential risks associated with the process, but one note of risk was observed. In addition to the aforementioned high temperatures of the reactor section, the reboiler on T-104 is operating at nearly 340 °C. This poses a safety hazard that will need to be evaluated using other safety techniques later on in the design process to minimize hazards. Additionally, sulfolane degradation occurs at 220 °C, this imposes a problem with recycling the sulfolane solvent.⁷ The degradation of sulfolane makes the solvent lose its

extraction properties and would therefore become ineffective. Sulfur dioxide and polymeric material are byproducts of sulfolane degradation, which are toxic and detrimental to process equipment.⁸ The binary coefficients in the liquid-liquid extractor will need to be examined in more detail for this process to be real-world applicable. Proper binary coefficients used for the simulation of the design could possibly resolve the issues with the high temperatures in the reboiler of T-104.

Process Safety Management

In order to prioritize safety and recognize any potential hazards, relevant data for all of the chemical constituents present within the process were collected and compiled. Safety data sheets (SDS) for each component were found from common industry employers and the necessary data was extracted and compiled. A summary can be seen below in Table 16.

With many of the components existing as a vapor at atmospheric temperature and pressure, the Occupational Safety and Health Administration (OSHA) permissible exposure limits for concentration during an 8-hour workday were collected. Air quality and ventilation systems should be tested regularly to ensure a safe environment for personnel within the plant. In areas of higher concentration, or heavy exposure, respiratory protection should be utilized. The high flammability of a majority of components within the process is another clear hazard. Although prevention of fires by identifying and minimizing any sources of ignition within the plant is a proactive approach, another layer of protection is added by developing firefighting and fire protection systems in case of an emergency. Personnel should be trained and aware of the unique firefighting measures found in SDS necessary to fight chemical fires. Fire retardant clothing should be worn by all personnel to protect from potential fire hazards. Additional personal protective equipment (PPE) should include safety glasses, hard hats, gloves, and chemical splash equipment when applicable.

Table 16: MSDS Summary⁹⁻²⁷

MSDS												
Component	Molecular Formula	Molecular Wt. (g/mol)	NFPA Diamond classifications				OSHA PEL TWA (ppm)	Oral Lethal Dose (LD ₅₀) (mg/kg)	Normal boiling point (°C)	Flash Point (°C)	Autoignition Temperature (°C)	Liquid Density (g/L)
			Health (blue)	Red (fire)	Yellow (reactivity)	White (special)						
Benzene	C₆H₆	78.12	2	3	0	none	1	2000 (Chevron SDS)	80	-11	498	0.88
Toluene	C₇H₈	92.15	2	3	0	none	200	6200 (Chevron SDS)	110.6	4.4	529	0.87
Xylene	C₈H₁₀	106.8	2	3	0	none	100	3426 (Chevron SDS)	138.3	27	528	0.86
Hydrogen	H₂	2	0	4	0	none	N/A	N/A (LC50 >15,000 ppm/hr Linde SDS)	-252.9	—	566	0.089
Methane	CH₄	16.04	2	4	0	none	1000 (ACGIH)	N/A (LC50 250,000 ppm/hr Matheson SDS)	-162	-223	537	0.717
Ethane	C₂H₆	30.08	1	4	0	none	1000 (similar to C ₁ -C ₃)	N/A (LC50 250,000 ppm/hr Matheson SDS)	-161.48	-104	287	—
Propane	C₃H₈	44.11	2	4	0	none	1000	—	-42.1	-104	287	—
Butane	C₄H₁₀	58	1	4	0	none	800	—	-0.5	-60	400	573
Pentane	C₅H₁₂	72.17	1	4	0	none	600	12,800 (Fischer Scientific SDS)	36	>-40	242.8	630
Hexane	C₆H₁₄	86.2	2	3	0	none	500	> 5000	67-69	-23	—	662.7
Heptane	C₇H₁₆	100.23	1	3	0	none	500	> 5000	98	-4	203.85	5.75
Octane	C₈H₁₈	114.26	2	3	0	none	500	> 5000	99	-12.22	411	0.69
Nonane	C₉H₂₀	128.2	3	3	0	none	200	> 5000	151	31	206	—
Decane	C₁₀H₂₂	142.28	1	2	0	none	N/A	> 5000	174	46	210	—
Cyclohexane	C₆H₁₂	84.16	2	3	0	none	300	> 5000	81	-18	260	779
Sulfolane	C₄H₈SO₂	120.18	1	1	0	none	N/A (0.37 Chevron SDS)	2143 (Chevron SDS)	100-286	166	—	1260
Napthalene	C₁₀H₈	128.17	1	3	0	none	10	N/A	218	80	526	—
Hydrogen Sulfide	H₂S	34.08	4	4	0	none	10	(LC50 712ppm/hr)	-60	—	270	—

A Piping and Instrumentation Diagram (P&ID) was completed for the largest distillation column within our process T-105 and is shown below in Figure 17.

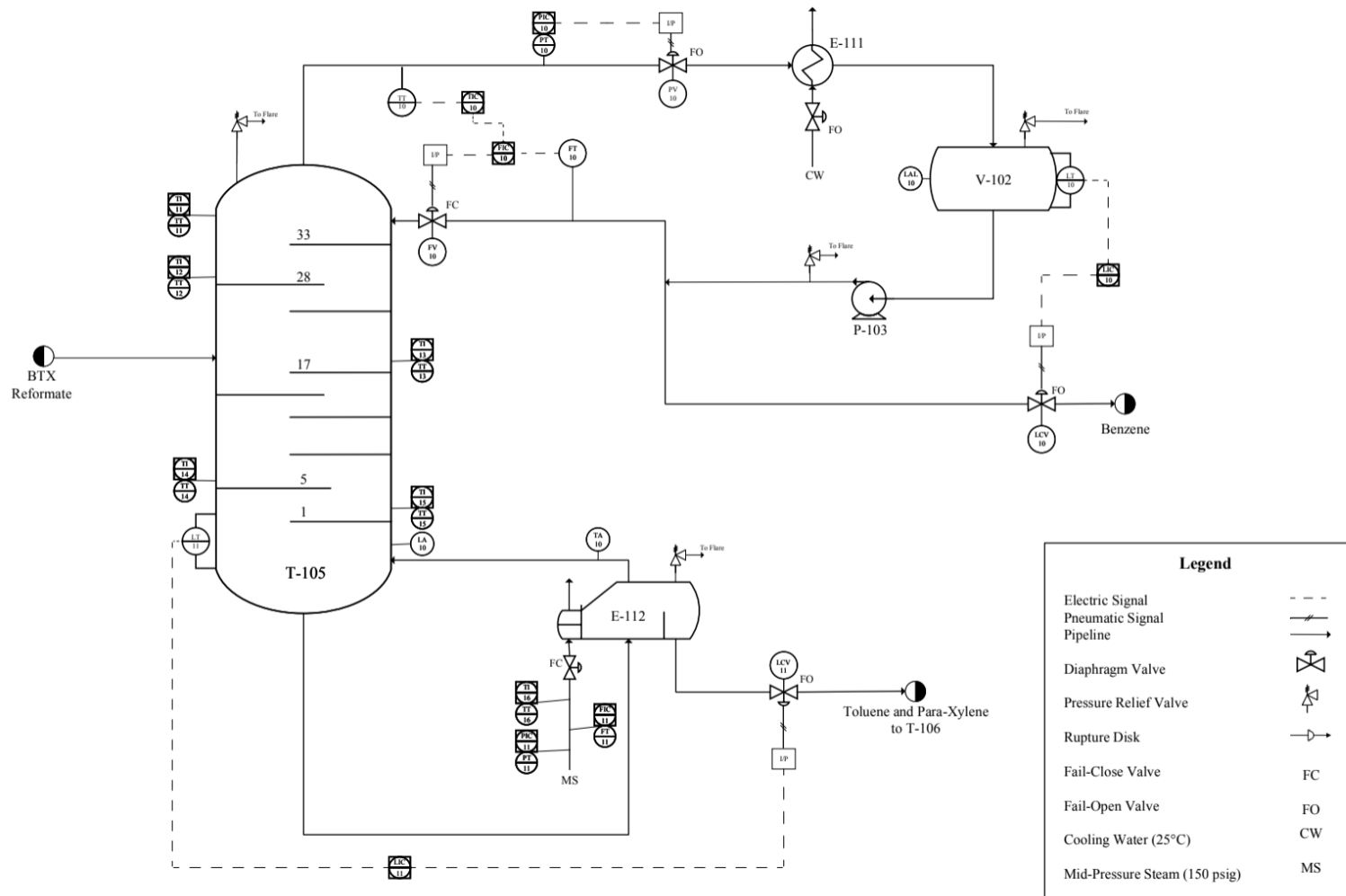


Figure 17: Major Fractionator P&ID

The major fractionator, T-105, employs numerous safety systems and control loops in order to ensure the safe and effective operation of the tower. T-105 has a sump level control loop in place to maintain the liquid level in the bottom of the tower. LT-11 reads the level of the liquid level and sends the signal to LIC-11. LIC-11 then calculates the flow rate needed to maintain the level of the sump by allowing the proper amount of flow through LCV-11. This loop ensures that the liquid level does not become too high or too low while operating the tower or during startup and shutdown. High levels will result in liquid entrainment and loss of purity, while low levels will result in the overheating of the reboiler and potentially result in running the tower dry. LA-10 will notify operators of a dangerous liquid level.

The reflux cascade control loop for the top of the tower uses the temperature reading from TT-10 to transmit a signal to the controller, TIC-10. This loop also maintains the reflux rate through FT-10, which transmits a signal to FIC-10. This reflux rate is directly related to the purity of the distillate, or the benzene product line. An increase in flow rate of reflux can cool the tower, as the reflux is condensed liquid received by the top stage of the tower. With both readings being taken into account, FIC-10 will ensure the temperature control and the reflux rate simultaneously. For this cascade loop, the temperature control is the master loop and the flow control is the slave loop. The overhead receiver, V-102, has a level control loop that is tied to LCV-10. The level is transmitted via LT-10, where LIC-10 calculates the needed flow rate through the liquid control valve, LCV-10. If the level of V-102 becomes too high, LIC-10 will determine how much flow should be increased to remove excess liquid from the vessel. In order to control the pressure of the tower, PC-10 takes the pressure reading and then transmits a signal to PIC-10, where the position of the valve PV-10 is calculated. The control loop determines the amount of flow needed to maintain the pressure of the top stage of the vessel. Pressure relief valves are placed strategically to prevent overpressure and to ensure the safe operation of each vessel. This mitigates the risk of an overpressure event of T-105, V-102, and E-112, as well as on the discharge of P-103. Each of these pressure safety valves are sent to a flare in the case of an overpressure event. This ensures that the excess flammable gases will be safely burned off to prevent them from becoming an explosion hazard if released from the equipment.

Alarms are strategically placed on certain areas of the system to inform operators of an event that could lead to equipment damage or physical harm to any employees or operators. TA-10 is placed on the outlet stream of the reboiler to provide warning of dangerously high temperatures of the reboiler. LA-10 is placed on the bottom of the tower to provide a warning of both high and low liquid levels in the sump. LAL-10 is placed on V-102 to warn of a low level in the vessel and prevent loss of the liquid seal, protecting from potential cavitation of P-103. Temperature indicators are placed on certain stages of T-105 to provide readings for operators to maintain proper operation of the tower.

A single spring-operated Pressure Relief Valve (PRV) was sized for T-105 for a non-fired scenario in accordance with API 520.²⁸ The mass flowrate of relief was estimated for a worst-case scenario, where the bottoms liquid was unable to be removed from the column due to a valve malfunction. With liquid feed still entering the column, the vapor space would decrease as the liquid level rose and overpressure in T-105 would ensue. The vapor relief rate required to prevent further pressure build up would therefore be equal to the flow rate out of the bottom during normal operation. The set pressure for the relieving device is equal to the maximum allowable working pressure (MAWP) since only a single relief device was used. The operating pressure is 90% of the MAWP. The accumulation pressure is 3 psi for vessels with set pressures between 15 and 30 psig.²⁸ The relieving fluid properties were simplified assuming benzene as the only component in the relieving vapor. The required relief area was found to be 16.1 cm². Orifice “L” was selected from API 526 with an actual relief area of 18.4 cm².²⁹ Three-inch pipe size for inlet and discharge piping to the relief valve allowed for reasonable pressure drop according to the ASME 3% and 10% rules. A summary is included, below, in Tables 17 and 18.

Table 17: PRV Sizing Pressures

	barg	bara
Operating Pressure	1.26	2.28
MAWP = Set Pressure	1.40	2.42
Pmax	1.61	2.62
Critical Flow Pressure (P*)	0.93	1.95
Delta P inlet (3% Set P)	0.04	1.06
Delta P Outlet (10% Set P)	0.14	1.15
Back Pressure	0	1.013

Table 18: PRV Sizing Data and Parameters

$k=C_p/C_v$ (Benzene)	1.12
Required Relief Rate (kg/hr)	6273
C (for $k=1.12$)	330
Temperature of Relieving Fluid (K)	381
MW (Benzene)	78.1
K_d	0.975
K_b	1.0
Actual Relief Rate (kg/hr)	7185
Required Area Relief (m ²)	0.00161
Actual Area relief (m ²)	0.00184
Orifice Designation	L

Another worst-case scenario that was explored, concerning T-105, would be a case where all of the liquid and vapor contents instantaneously vaporize, vent to the atmosphere, and ignite. A TNT equivalency calculation was performed to determine the blast radius and extent of damage to objects and structures at varying distances. The vapor cloud explosion (VCE) was determined to have an equivalent mass of 141kg of TNT. An explosion efficiency of 10% was used in the calculation for a conservative estimate, with typical values ranging from (1-10)%³⁰. The over pressure was determined at varying distances from the explosion which correlates with the extent of damage.

Due to the nature of VCEs this method tends to overestimate the overpressure closer to the explosion and underestimate the overpressure at greater distances from the explosion. Our conservative explosion efficiency was expected to account for these differences. In Figure 18 below, the blast radius is mapped with damage as a function of distance from the explosion. These distances should be heavily considered with plant siting.

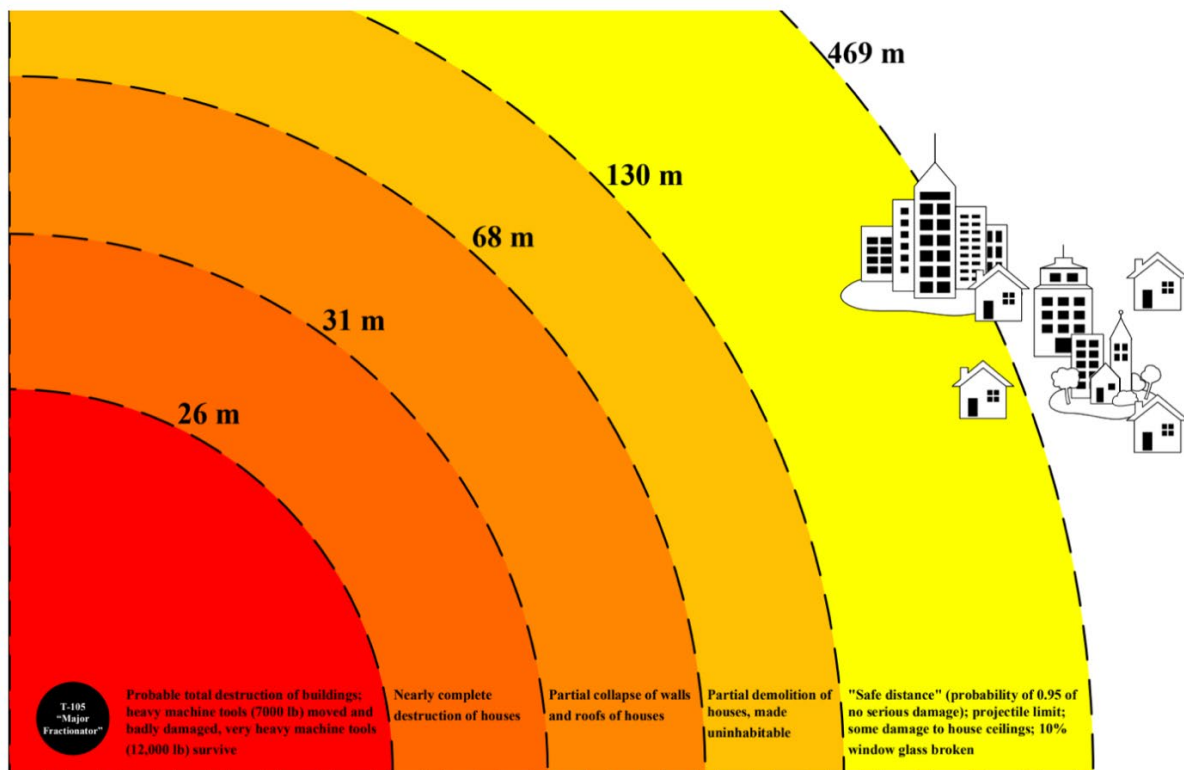


Figure 18: Blast Radius Map

In addition to this VCE simulation, the upper and lower explosion limits of the expected vapor mixture were calculated and are summarized below in Table 19.

Table 19: Lower Explosion Limit (LEL) and Upper Explosion Limit (UEL) Values

Component	Formula	(vol % fuel in air)	
		LEL	UEL
Benzene	C6H6	1.50	9.54
Toluene	C7H8	1.25	7.98
p-Xylene	C8H10	1.08	6.87
Mixture	—	1.34	8.54

In hopes of considering all possible scenarios and mitigating risk, a “What If?” hazard analysis was completed for T-105 and the subsequent control system. The analysis is summarized in Table 20 below. Human and procedural errors were determined to be the greatest risk for safety within the plant. As such, the attitude towards safety and adequate training should be paramount in day-to-day operation.

Table 20: Worst-case Scenario Summary

Hazardous Event/Scenario	Hazard Mechanism/Outcome	Likelihood	Consequence(s)	Lines of Defense	Hazard Rating/Risk Analysis	Recommended Action
Failure of Reflux P-103	Over heating of T-105	Unlikely	Process Upset	Spares	Low	None
Loss of instrument air	Pneumatic Valves default to failure position	Unlikely	Process Upset	PRV, Valve fail position design	Low	None
Failure of Level Control in T-105	Possible Over Pressure in T-105	Unlikely	Process Upset	Level Alarms, PRV	Low	None
Loss of Cooling Water	Over Pressure in T-105	Unlikely	Process Upset	PRV	Low	None
Fire in plant	Over Pressure in T-105	Unlikely	Plant Shutdown	None	Medium	Install fire fighting measures
Elevated Feed Temperature into T-105	Eventual overpressure in T-105	Unlikely	Process Upset	Process Control System and Temperature Indicators	Low	None
Error in Startup and/or Shutdown Procedures	Tower operating in a manner not according to design	Likely	Process Upset	Training, SIFs	High	Ensure training on safety and procedures is routine and thorough
Un-managable overpressure T-105	Pressure Vessel Burst	Very Unlikely	Toxic Release, explosion, loss of life	PRV, Low vessel operating pressure	Low	Siting of plant in remote area and/or Emergency Respose Planning
Error in Operating Procedures	Tower operating in a manner not according to design	Likely	Process Upset	Training, SIFs	High	Ensure training on safety and procedures is routine and thorough
Failure of engineering controls to prevent harmful levels of toxic vapor	Harmful to employees, contractors, and personnel in the plant	Unlikely	Injury and possible loss of life	Adequate ventilation and PPE in place	Low	None

Safety Summary

Safety considerations are paramount to the design of any process to ensure protection from incident and catastrophe for the plant staff, nearby residents, and the environment. Engineers have an obligation to the local community to mitigate as much risk as possible. An aim of this design is also to meet Western standards of safety.

Inherently safer design practices for this unit limited risk by opting for low operating pressures and temperatures, substituting heat exchange mediums for less hazardous options, as well as reducing the quantity of equipment. Process safety management (PSM) of the design consisted of a process hazard analysis, consideration for controls equipment on the major fractionator, T-105, and an in-depth worst-case scenario analysis. The TNT equivalence, a pressure safety valve (PSV), and UEL and LEL were calculated as part of the PSM. TNT equivalence is summarized with the blast radius map in Figure 18. The diameter of the PSV was determined to be 5.25 cm and the explosive limits of the mixture was 1.34-8.54 volume %. The P&ID of T-105 illustrates the implementation of control loops to prevent unsafe process conditions, such as high temperatures, overpressure, and fluctuations of process flow rates. Alarms are included in the highest risk areas of the unit. Fail-safety positions of valves are designated on the P&ID to ensure proper redirection of process and energy streams to prevent unsafe conditions in the case of a power-loss to the system. A “What-If” analysis covers any circumstances where danger in the plant can arise, so that consequence of incidence can be reduced through emergency response procedure.

Conclusions

The Toppings Refinery Retrofit design employed strategies of optimization, inherent safety design, and cost-effective solutions to ensure safe processing of hazardous components from both feeds, K and TQ1. Safe processing of these feeds resulted in revenue generating streams of salable benzene, toluene and para-xylene, as well as gasoline and diesel products. The proposed design was projected to be profitable for both feeds under both the Iraqi and Kurdish tax regimes, with NPV exceeding \$100 Million for all cash flow scenarios investigated. Feed TQ1 under the Kurdish tax regime reported the greatest NPV and DCFROR of approximately \$330 Million and 114%, respectively. The lowest calculated DCFROR among the scenarios was for Feed K under the Iraqi tax regime with a value of 57%. Overall, the design resulted in greater profitability from the

processing of Feed TQ1, when compared to Feed K. Payback periods between the two feeds and tax regimes varied between 1 year, 7 months and 2 years, 4 months. The payback period averaged a length of 2 years between the scenarios. High NPVs and DCFRORs were seen between the feed and tax regime options investigated, even under worst-case single-parameter sensitivity analyses. For the reasons previously listed, the proposed retrofit design is recommended to be pursued further with relatively low risk.

A few considerations moving into the detailed design phase of the proposed design include further safety investigations and optimization strategies. Foremost, the high temperature of the reboiler FH-103, recovering the sulfolane solvent, must be further investigated. Adjustment of the binary coefficients in Aspen HYSYS could possibly aid with these conditions and should be investigated to resolve the issue of potential solvent degradation. Another recommended strategy to improve safety and optimization of the process is to consider the influence of divided wall columns as a minimization strategy. Implementing this distillation column design could greatly reduce capital and manufacturing costs of distillation towers, as well as reduce consequence of incidents and risk.

Appendix

A. Reactor Train Detail

Table 21 shows that the equipment for the reactor section will cost \$5.4 Million. This is mainly comprised to the cost of the first fired heater in series and the compressor. These two pieces of equipment also demand the most of the \$7.7 Million annual utility costs.

Table 21: Reaction Section Summary

Reactor Section Cost Summary			
Tag	Description	Bare Module Cost	Annual Utility Cost
C-100	Hydrogen Recycle Compressor	\$1,950,000	\$1,210,000
E-100	Naphtha Feed Preheater	\$160,000	\$0
E-101	Stream 11 Cooler	\$220,000	\$170,000
FH-100	Fired Heater 1	\$1,340,000	\$2,900,000
FH-101	Fired Heater 2	\$720,000	\$140,000
FH-102	Fired heater 3	\$720,000	\$160,000
P-100	Naphtha Feed Pump	\$130,000	\$70,000
R-100	Reactor 1	\$20,000	--
R-101	Reactor 2	\$40,000	--
R-102	Reactor 3	\$40,000	--
R-103	Swing Reactor	\$40,000	--
V-100	Hydrogen Vapor Separator	\$50,000	--
Reactors	Reactor Catalyst	--	\$3,000,000
Labor	Operating Labor Cost	--	\$90,000
Total		\$5,430,000	\$7,740,000

The catalytic reformer train section includes a series of three reactors, R-100, R-101, and R-102, alternated with fired heaters FH-100, FH-101, and FH-102. An integrated heat exchanger, E-100, is implemented before the first reactor. Cracking and dehydrogenation reactions, detailed by equations 1, 2, 3, and 4, are performed in this series of reactors to produce shorter alkane products from long carbon chains in the naphtha feed, as well as produce benzene through the dehydrogenation of cyclohexane in the feed. These reactions are endothermic, thus requiring fired heaters to heat the process stream back up to the reaction temperature before entering the next subsequent reactor.

Each reactor was modeled as a fixed bed reactor, containing a platinum catalyst on a silica base. Carbonaceous coke deposits and residue reduce the availability of active sites on the catalyst, reducing catalyst activity.³¹ Catalyst must be removed and regenerated, or replaced, approximately every 6 months to maintain reaction performance. Annual spending on the replacement and regeneration of platinum catalyst is estimated to be \$3 million.³² Considering that catalyst must be regenerated routinely, a swing reactor, R-104, is employed to ensure that the catalytic reforming

unit can continue production, preventing process shutdown, while servicing and replacing the catalyst. This is achieved by regenerating the catalyst in situ, where the swing reactor replaces the function of any given reactor as it is out of service, maintaining a series of three reactors to avoid shutdown and continue operation. This type of reactor train is referred to as a cyclic catalytic reformer.

Reactor conditions, such as temperature, pressure drop, volume, and void fraction of catalyst, were modeled after Iranshahi, D., *et al.* as a starting point for reference.² Adjustments to the reaction train conditions were made from this reference point by observing product yields in the Aspen HYSYS simulation. Pressure drop across the reactors R-100, R-101, and R-102, were 0.7, 0.6, and 0.4 bar, respectively. The process stream was heated to 438°C for the inlet of each reactor. The void fraction for the platinum catalyst was 0.38. The hydrogen ratio for this process was also influenced by Iranshahi, D., *et al.*, but was optimized from an 80% recycle to 90% based on Aspen HYSYS simulation outputs.²

The kinetic energies for the catalytic cracking and dehydrogenation reactions in this process follow the general equation:

$$k = Ae^{-\frac{E_a}{R}} P_x \quad (5)$$

where P_x is the partial pressure of the reactant(s), x , A is the pre-exponential factor, E_a is the activation energy, and R is rate constant ($8.314 \frac{\text{Joule}}{\text{mol} \cdot \text{Kelvin}}$). Kinetic parameters in Table 22 include pre-exponential factors, A , and the activation energies, E_a , of the reactions. Reactions 1 and 4 are reversible and are expressed with two terms, the positive to describe the forward reaction kinetics and the negative term for the reverse. The negative effective activation energy in Reaction 1 indicates the complexity of reaction steps involved in use of a catalyst. Binding to active sites on the catalyst adds steps to the reaction sequence and composite elementary effective activation energies can sum to result in a negative value³³.

Table 22: Table of Kinetic Parameters for Reactions 1-4

	Pre-Exponential Factor, A	Activation Energy, E _a [J/mol]
Reaction 1 (Fwd)	9.4928 x 10 ¹³ hr ⁻¹	160506.4
Reaction 1 (Rev)	8.2728 x 10 ⁻⁴ hr ⁻⁴	-52170.4
Reaction 2	3.6703x10 ²¹ hr ⁻¹	287756.8
Reaction 3	3.6704x10 ²¹ hr ⁻¹	287756.8
Reaction 4 (Fwd)	3.33674x10 ¹⁹ hr ⁻²	275285.8
Reaction 4 (Rev)	4.19816x10 ²¹ hr ⁻¹	312237.9

An innovative design implemented in the reaction train section was the use of an integrated heat exchanger which used the exiting process fluid to heat the incoming feed stream prior to entering the first fired heater, FH-100. This innovation in the design of the catalytic reformer reduces the heat duty and fuel gas supply required by FH-100, as well as reduces the cooling water flow required by stream cooler E-101. For this reason, the heat-integrated heat exchanger, E-100, reduces annual utility costs and efficiently transfers heat energy between the streams.

B. Extractor Section Detail

Below, in Table 23, the extraction section costs are summarized. A total of \$9.6 Million is required for purchasing the equipment and \$9.8 Million is required to operate the equipment annually. The reboiler on T-104, FH-103, has a notable annual utility expense, and as aforementioned would need reevaluation in a more detailed process design.

Table 23: Extraction Section Summary

Extraction Section Cost Summary			
Tag	Description	Bare Module Cost	Annual Utility Cost
E-102	T-100 Reboiler	\$130,000	\$240,000
E-103	Stream 22 Cooler	\$200,000	\$20,000
E-105	Stream 27 Cooler	\$120,000	\$30,000
E-106	Stream 29 Cooler	\$280,000	\$50,000
E-107	Stream 35 Cooler	\$100,000	\$0
E-108	Stream 41 Cooler	\$120,000	\$0
E-109	T-103 Reboiler	\$210,000	\$240,000
E-115	Sulfolane Recycle Cooler	\$930,000	\$400,000
FH-103	T-104 Reboiler	\$2,480,000	\$8,620,000
P-101	T-103 Feed Pump	\$30,000	\$10,000
P-102	T-103 Feed Pump	\$70,000	\$900
P-106	Sulfolane Recycle Pump	\$190,000	\$70,000
T-100	T-100 Tower	\$80,000	--
T-101	T-101 Extraction Tower	\$190,000	--
T-102	T-102 Extraction Tower	\$40,000	--
T-103	T-103 Tower	\$130,000	--
T-104	T-104 Tower	\$4,230,000	--
V-101	Recycle Vapor Separator	\$20,000	--
Labor	Operating Labor Cost	--	\$140,000
Total		\$9,550,000	\$9,820,900

The aim of the extraction section was to isolate linear alkanes into a stream of C1-C4s, for use in the plant, salable C5-C8s as gasoline and diesel product, and to purify the BTX Reformate to at least 99%. The process set-up for the extractor section was modeled after the works of Blahušiak, M., *et al.*³⁴ T-100, the first stripper in the section removes light alkanes in its top product. The bottoms stream is then sent to be processed through a series of two extractor units. These extraction units were used to extract benzene from the gasoline and diesel product. A 4-to-1 ratio between the sulfolane solvent and process feed was used to extract the benzene from the gasoline and diesel product. The second extractor runs extraction water to remove sulfolane from the final salable gasoline and diesel. BTX Reformate, modeled from “benzene”, is separated from water as well as other linear alkanes in the final stripping column, T-103. This BTX Reformate is then sent to the distillation section.

Stripper T-104 of the extraction section is notable for separating pure sulfolane from the water and benzene, and some remaining linear alkanes. This piece of equipment allows for the sulfolane solvent to be recycled. Recycling the sulfolane proved to be economically favorable, as no profit was seen without it. Approximately \$6.6 Billion would be spent annually on the continuous feed of sulfolane, in the case a recycle was not implemented.

Using the provided PFD for the original design of the toppings unit, it was determined that the use of strippers and a series of recycles was a better fit for the needed purity of benzene production as reformat. Using the same layout for the initial stripper and extraction section, products from both extractors, T-101 and T-102, were sent to a stripper, T-104, to separate the sulfolane. The initial extractor design uses pure sulfolane, however it was found that using 0.5% water mix with the sulfolane solvent creates a better environment for benzene extraction. The bottoms product of T-104, sulfolane, is sent back to the extractor T-101 for a recycle and the lighter components are sent to a vapor separator, V-101, where the bottoms products are sent to the reformat producing stripper, T-103, replacing the use of a distillation column. V-101 top product was recycled back to the bottom inlet of extractor T-101. The principle use of the vapor separator is to remove the excess butane from the water and the benzene products. T-103 is used to remove any excess water from the benzene as a top product, as well as any linear alkanes, and is sent back into the sulfolane extractor. This proves to create a more efficient cycle for producing benzene, at a purity of 99.82%, from the bottoms of T-103. Additionally, the process feed into the first extractor, T-101, was designed to enter on the 15th stage. This was an effective design that resulted in greater extraction results from T-101.

C. Distillation Section Detail

The distillation section cost summary is provided below in Table 24, reporting a total bare module cost of the equipment of \$1.62 Million and annual utility costs of \$450,000. The largest capital expense within the section was the reboiler, E-114, which costed \$440,000. For annual utility costs, the greatest amount of annual spending for this section was allocated to the reboiler of T-105 at \$170,000.

Table 24: Distillation Section Summary

Distillation Section Cost Summary			
Tag	Description	Bare Module Cost	Annual Utility Cost
E-110	Feed Cooler	\$110,000	\$10,000
E-111	T-105 Condenser	\$90,000	\$20,000
E-112	T-105 Reboiler	\$200,000	\$170,000
E-113	T-106 Condenser	\$90,000	\$30,000
E-114	T-106 Reboiler	\$440,000	\$140,000
P-103	T-105 Reflux Pump	\$30,000	\$2,000
P-104	T-106 Feed Pump	\$30,000	\$1,000
P-105	T-106 Reflux Pump	\$30,000	\$5,000
T-105	T-105 Tower	\$220,000	–
T-106	T-106 Tower	\$330,000	–
V-102	T-105 Overhead Receiver	\$20,000	–
V-103	T-106 Overhead Receiver	\$30,000	–
Labor	Operating Labor Cost	--	\$70,000
Total		\$1,620,000	\$448,000

The distillation section of the naphtha processing unit is responsible for taking in BTX Reformate and producing the salable three product streams from the two distillation columns. The instantiated reformate, composed of benzene, toluene, and para-xylene, is introduced to the distillation section where the components will be separated based on their relative volatilities. Distillation columns separate the most volatile components through their top product streams. The first column in the series separates benzene and sends it out through the top stream of the column. Toluene and para-xylene are sent through the bottoms stream to the next distillation column. In T-106, toluene is sent out of the column as the top stream product and para-xylene is separated into the bottom stream.

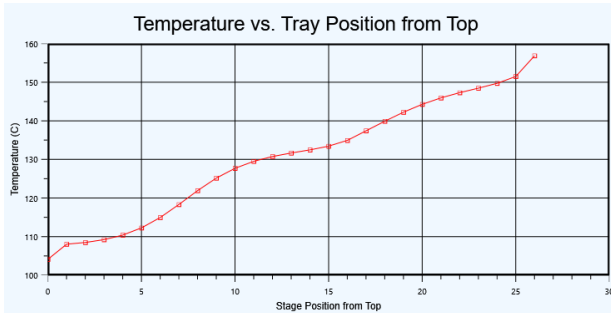


Figure 19: Temperature Profile of T-105

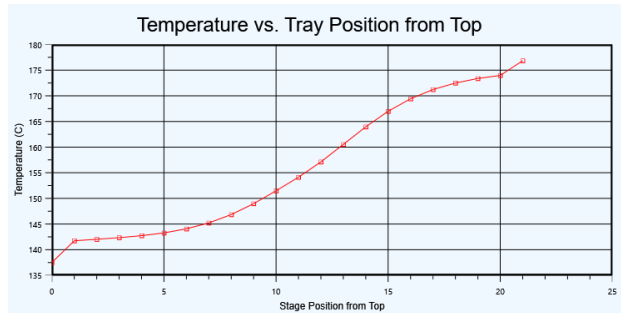


Figure 20: Temperature Profile of T-106

Temperature profiles for distillation columns T-105 and T-106 are displayed above as figures 19 and 20. The charts illustrate the temperature increase with respect to theoretical stage position, numbered from the top of the column. The lowest temperatures in the columns occur at the top, where condensate from the overhead receiver is sent back to the top stage in a liquid phase. Temperatures increase down the height of the column, as the heated stream from the top of the reboiler is sent back into the tower at the bottom stage.

D. Equipment Sizing

Below in Tables 25 through 32 detail sizing data for the equipment in the process is provided. This includes specifications of the designs such as material of construction, parameters used to size and cost, capacities of the equipment and energy data.

Table 25: Column Detail Sizing and Specifications

Column Details								
Sizing Summary					Materials of Construction			
Title	Internals	Number of Theoretical Trays	Diameter [m]	Volume [m ³]	Construction Material	Nominal Packing Type	Tray Type	Internal Material
T-100	Packed	10	1.07	8.17	Carbon Steel	2 in Pall Rings	–	Metal (304SS)
T-103	Packed	20	1.07	13.62	Carbon Steel	2 in Pall Rings	–	Metal (304SS)
T-104	Packed	12	3.96	127.79	Nickel Alloy	2 in Pall Rings	–	Metal (304SS)
T-105	Trayed	25	0.91	15.21	Stainless Steel	–	Sieve	Carbon Steel
T-116	Trayed	20	1.22	46.26	Carbon Steel	–	Sieve	Carbon Steel

Table 26: Vapor Separator Sizing Details and Specifications

Vessel Details				
Title	V-100	V-101	V-102	V-103
Orientation	Vertical	Vertical	Horizontal	Horizontal
Vapor Mass Flow [lbm/hr]	6.79E+04	4.30E+04	0.00E+00	0.00E+00
Liquid Mass Flow [lbm/hr]	7.27E+04	2.11E+04	2.60E+04	4.06E+04
Vapor Density [lbm/m ³]	18.32	8.57	12.37	13.38
Liquid Density [lbm/m ³]	1506.17	1942.31	1725.12	1657.32
Density of Mixture [lbm/m ³]	37.43	12.74	–	–
Diameter [m]	2.29	1.98	1.07	1.22
Volume [m ³]	16.26	8.93	4.78	6.98
Construction Material	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel

Table 27: Reactor Sizing Details and Specifications

Reactor Details		
Title	Volume [m ³]	Construction Material
R-100	11.33	Carbon Steel
R-101	14.16	Stainless Steel
R-102	16.99	Stainless Steel
R-103	16.99	Stainless Steel

Table 28: Compressor Sizing Details and Specifications

Compressor Details			
Title	Type	Brake Horsepower	Construction Material
C-100	Centrifugal	700	Stainless Steel

Table 29: Heat Exchanger Sizing Details and Specifications

Heat Exchanger Details									
Materials of Construction					HEX Sizing Summary				
Title	Description	Type	Tube Material	Shell Material	Total Q [BTU/hr]	Approach Temperature	Overall Heat Transfer Coefficient [BTU/hr*ft ² *°F]	LMTD [°C]	Surface Area [m ²]
E-100	Heat Integrated Stream 3 Heater	Floating Head	Carbon Steel	Carbon Steel	3.39E+07	291.00	72.76	160.32	149.97
E-101	Stream 11 Cooler	Floating Head	Carbon Steel	Carbon Steel	3.78E+07	23.00	119.33	51.21	263.48
E-102	T-100 Reboiler	Kettle Reboiler	Carbon Steel	Carbon Steel	5.33E+06	142.40	200.00	74.77	16.50
E-103	Stream 22 Cooler	Floating Head	Carbon Steel	Carbon Steel	4.51E+06	4.51E+06	37.79	12.24	227.96
E-105	Stream 27 Cooler	Floating Head	Carbon Steel	Carbon Steel	6.55E+06	97.30	69.25	41.32	91.72
E-106	Stream 29 Cooler	Floating Head	Carbon Steel	Carbon Steel	1.11E+07	23.00	64.63	9.00	369.11
E-107	Stream 35 Cooler	Floating Head	Carbon Steel	Carbon Steel	2.84E+05	23.00	47.29	9.00	12.86
E-108	Stream 41 Cooler	Floating Head	Carbon Steel	Carbon Steel	5.62E+05	23.00	118.00	29.02	5.84
E-109	T-103 Reboiler	Kettle Reboiler	Carbon Steel	Carbon Steel	5.47E+06	77.80	200.00	24.75	36.88
E-110	Stream 47 Cooler	Floating Head	Carbon Steel	Carbon Steel	2.28E+06	257.00	112.96	128.03	7.92
E-111	T-105 Condenser	Floating Head	Carbon Steel	Carbon Steel	4.32E+06	142.40	150.00	60.53	21.07
E-112	T-105 Reboiler	Kettle Reboiler	Carbon Steel	Carbon Steel	3.83E+06	61.30	200.00	13.54	35.06
E-113	T-105 Condenser	Floating Head	Carbon Steel	Carbon Steel	6.16E+06	202.50	150.00	94.05	21.07
E-114	T-106 Reboiler	Kettle Reboiler	Carbon Steel	Carbon Steel	3.13E+06	20.80	200.00	-7.71	89.16
E-115	Stream 69 Cooler	Floating Head	Nickel Alloy	Nickel Alloy	9.12E+07	18.00	112.96	67.08	545.73

Table 30: Fired Heaters Sizing Details and Specifications

Fired Heaters Details			
Title	Description	Duty [hp]	Design Pressure [bar]
FH-100	1 in Reactor Series	1.45E+04	15.34
FH-101	2 in Reactor Series	7.22E+02	14.65
FH-102	3 in Reactor Series	8.01E+02	13.10
FH-103	T-104 Reboiler	4.32E+04	5.74

Table 31: Liquid-Liquid Extractor Sizing Details and Specifications

Liquid-Liquid Extractors Details					
Title	Number of Trays	Diameter [m]	Tray Spacing [m]	Volume [m3]	Construction Material
T-101	30	1.52	0.50	27.36	Nickel Alloy
T-102	20	1.52	0.50	18.24	Carbon Steel

Table 32: Pump Sizing Details and Specifications

Pump Details							
Title	Supply Pressure [bar]	Feed Pressure [bar]	Liquid Density [lb/m ³]	Feed Stage	Feed Stage [m ³ /hr]	Drive Capacity [hP]	Purchased Power [hP]
P-100	1.20	11.03	1544.31	0	65.24	40	44.44
P-101	1.79	4.89	1911.23	10	10.77	3	3.33
P-102	4.69	4.83	1982.21	20	0.3331	0.5	0.56
P-103	2.07	2.28	1725.12	25	0	1	1.11
P-104	2.59	2.35	1612.82	11	7.189	0.75	0.83
P-105	2.07	2.28	1657.32	20	17.02	3	3.33
P-106	2.15	6.62	2748.54	0	124.7	40	44.44

References

1. **Kent, J. A. (Ed.)**, "Riegel's Handbook of Industrial Chemistry," Springer, Manhattan, NY (2003).
2. **Iranshahi, D., et al.**, "Applying New Kinetic and Deactivation Models in Simulation of a Novel Thermally Coupled Reactor in Continuous Catalytic Regenerative Naphtha Process," *Chemical Engineering Journal*, pp. 154-164 (2013).
3. **Askari, A., et al.**, "Simulation and Modeling of Catalytic Reforming Process," *Petroleum & Coal*, pp. 77-79 (2011).
4. **Turton, R., et al.**, "Analysis, Synthesis, and Design of Chemical Processes," 4th ed., *Prentice Hall*, pp. 161-263 (2017).
5. **McHone Industries**, "A Guide to Carbon Steel Grades," <https://blog.mchoneind.com/blog/carbon-steel-grades-chart> (2017).
6. **U.S. Bureau of Labor Statistics**, "Current Employment Statistics," available online at <https://www.bls.gov/ces/>, Washington, DC
7. **Chevron Phillips Chemical Co.**, "Specialty Chemicals- Sulfolane," available online at www.cpchem.com/specialtychemicals, The Woodlands, TX.
8. **U.S. Environmental Protection Agency**, "Sulfur Dioxide Basics," available online at <https://www.epa.gov/so2-pollution/sulfur-dioxide-basics>
9. **Sigma Aldrich Co.**, "Material Safety Data Sheet- Naphthalene," Version 5.2 (2013).
10. **Sigma Aldrich Co.**, "Material Safety Data Sheet- Cyclohexane," Version 5.1 (2013).
11. **Thermo Fisher Scientific**, "Safety Data Sheet- Decane," Revision 4 (2010).
12. **Thermo Fisher Scientific**, "Safety Data Sheet- n-Nonane," Revision 4 (2010).
13. **Airgas**, "Safety Data Sheet- Hydrogen Sulfide," Version 1.01, Radnor, PA (2017).
14. **Airgas**, "Safety Data Sheet- Propane"
15. **Airgas**, "Safety Data Sheet- Ethane"
16. **Airgas**, "Safety Data Sheet- Flammable Liquid Mixture: Benzene/Heptane/Hexane/Octane/ P-Xylene/Sulfolane/Toluene"
17. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Octane," Version 1.7, The Woodlands, TX.
18. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Heptane," Version 1.1, The Woodlands, TX.
19. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Hexane," Version 1.5, The Woodlands, TX.
20. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Pentane," Version 1.5, The Woodlands, TX.
21. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Para- Xylene," Version 1.7, The Woodlands, TX.
22. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Toluene," Version 1.7 The Woodlands, TX.
23. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Benzene," Version 1.9, The Woodlands, TX.
24. **Chevron Phillips Chemical Co.**, "Safety Data Sheet- Sulfolane," Version 2.3, The Woodlands, TX.
25. **Praxair Inc.**, "Butane n- Safety Data Sheet P-4572," Danbury, CT (2016).
26. **Praxair Inc.**, "Hydrogen, compressed- Safety Data Sheet P-4604," Danbury, CT (2016).
27. **Matheson**, "Safety Data Sheet- Methane," Revision 1, Basking Ridge, NJ (2009).
28. **American Petroleum Institute**, "Sizing, Selection, and Installation of Pressure-relieving Devices," API Standard 520, 9th ed., Washington, DC (2014).
29. **American Petroleum Institute**, "Flanged Steel Pressure Relief Valves," API Standard 526, 5th ed., Washington, DC (2002).
30. **Crowl, D.A., and J.F. Louvar**, "Chemical Process Safety: Fundamentals with Applications," 3rd ed., Pearson Education, Westford, MA (2011).
31. **Eser, S.**, "Continuous Catalyst Regeneration," available online at <https://www.e-education.psu.edu/fsc432/content/continuous-catalyst-regeneration>, College of Earth and Mineral Sciences, PennState, University Park, PA (2020).
32. **Valero**, Finances Department, contacted on 3/29/21, San Antonio, TX.
33. **Physical Chemistry Chemical Physics**, "A time to search: finding the meaning of variable activation energy," available online at www.rsc.org/pccp, Volume 18, p. 18617-19484, Royal Society of Chemistry (2016).
34. **Blahušiak, M., et al.** "Insights into the selection and design of fluid separation processes," **194**, p. 301-318, "Separation and Purification Technology" (2018).