Letter of Transmittal

April 14, 2021
Mr. Abbasi
Kirkuk Iraq
AICHE Student Design Competition

To Whom It May Concern:

Within the attached report, you will find a preliminary design for the Toppings Refinery Retrofit for Mr. Abbasi in Kirkuk, Iraq. The feasibility of the project is contained within the report.

The preliminary design includes a simulation which will internally expand the toppings refinery Mr. Abbasi runs. The design contains a process description as well as flow diagrams of the proposed design, analysis of the economic feasibility of the proposition, and the design's overall process safety summary. The proposed design possesses the ability to process both requested crude oil supply streams.

Thank you for the opportunity to complete this preliminary design. Your partnership is appreciated, and we look forward to working with you in the future. If you have any questions upon review of the report, feel free to reach out to the design team.

Regards,

The Process Design Team

Spring 2021

AIChE Student Design Competition

Toppings Refinery Retrofit
Kirkuk, Iraq

Executive Summary

In response to heightened pressure to meet western refining standards from local governments, the toppings refinery unit in Kirkuk, Iraq must be updated. The redesign and construction of this facility will incur costs in year 2021 with full production beginning by mid-year 2022. The facility will be able to process naphthas from local light sweet crudes at a capacity of 35,000 BPD. The facility will produce chained hydrocarbon, benzene, para-xylene, and toluene product streams. The chained hydrocarbon product will be utilized for gasoline and diesel sales. These products were achieved through use of a fired heater utilizing natural gas as fuel, three reactors for "cracking" naphtha feedstock into components useful for fuel, two extractors utilizing sulfolane and water to extract chained hydrocarbons, and five distillation columns: a tower to remove C_4H_{10} and lighter, a tower following the first extraction tower removing carry over sulfolane, a tower to isolate the reformate of benzene, toluene, and para-xylene, and two more towers to further separate these three components. Heat exchangers, pumps, separator vessels, and a compressor were also utilized as necessary for this process. The facility holds enough capacity to process two common feeds from the Kirkuk region; however, the main feed of interest was given greatest consideration in optimization. Hydrocarbon product streams reach up to 74,200 lb/hr; benzene product streams reach up to 5,160 lb/hr; toluene product streams reach up to 3,370 lb/hr, and para-xylene product streams reach up to 2,410 lb/hr.

Capital costs necessary for purchasing and installing all equipment in 2021 totaled around $151 million. Yearly operating costs for the facility, assuming a service factor of 0.92, total $31.8 million for the feedstock of interest which includes full compensation for 16 operators, incurring a labor cost of $217,000 annually. The feedstock of interest costs $287 million when including naphtha, sulfolane, and process water costs.

Annual revenue for the key feed stream totals around $805 million annually. Taxes greatly affect the annual profit; two different tax regimes were necessary to consider for this project. Iraqi taxes at 35% cause less profit to be earned than Kurdish taxes at 15%. If Iraqi taxes are considered, the process has an expected net present value of $594 million, a discounted cash flow rate of return of 115%, and a discounted payback period of 1.29 years under a 5-year project evaluation life with a 15% hurdle rate. Under Kurdish taxes, the process has an expected net present value of $797 million, a discounted cash flow rate of return of 143%, and a discounted payback period of 1.10 years under a 5-year project evaluation life with a 15% hurdle rate. Escalation of raw material costs and reduced profit provide the greatest risk to the economic success of the project. Under variable analysis, Iraqi taxes showed a 79.6% chance to have a net present value greater than 0 with Kurdish taxes doing better at an 84.8% chance of the same result.

After analyzing the provisional process flow diagram, our team decided to remove the column directly following the second extractor which would have provided an additional sulfolane recycle stream leaving the bottoms. The elimination of this column provided for an inherently safer design and more lucrative project economics. The project team utilized numerous other safety features as necessary. No factor was given greater consideration than process safety.

It is the design team's conclusion that this project is economically attractive; therefore, it is our recommendation that the project be evaluated for detailed design and considered for prompt construction.

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Process Description

Our process is modeled with one incoming feed stream that could have two separate compositions. The primary composition is feed K while the secondary composition is feed TQ1. These flow rates for feeds K and TQ1 are 7,000 BPD and 9,800 BPD, respectively. Compositions of each feed are given below in Table 1.

Table 1: Feed Compositions

	K	TQ1
Specific Gravity	0.749	0.7308
n-Decane mol%	59.7	77.8
Cyclohexane mol%	31.3	20.6
Benzene mol%	9	1.6

The feed (stream 1) is pumped into a fired heater (F-101) at 230.4^{o}F and 100 psia before being fed (stream 4) into the first reactor, R-101. The products leaving the reactor (stream 5) are fed back into the fired heater and used as feed (stream 6) into R-102. This process is repeated in R-102 as its products are fed (stream 7) back into the heater and used as feed (stream 8) for R-103. The product stream leaving R-103 (stream 9) is cooled through a floating head heat exchanger (E-102) and fed (stream 10) into a vapor liquid separator (V-101). The goal of these three reactors is to "crack" the heavier n-decane and cyclohexane components into smaller chain alkanes. Reaction kinetics for these components are given below in Table 2. Rates are in terms of kmol/(m^3-hr), pressures in MPa, and temperature in Kelvin.

Table 2: Reaction Rates

Reaction	Rate
$C_6H_{12} \rightarrow C_6H_6 + 3H_2$	$(9.4928*10^{13})\ e^{-160506.4/(8.314T)}\ P_{C6H12} - (8.2728*10^{-4})e^{52170.4/(8.314T)}P_{C6H6}P_{H2}^3$
$C_6H_{12}+2H_2 \rightarrow 0.4C_5H_{12}+0.4C_4H_{10} +0.4C_3H_8+0.4C_2H_6+0.4CH_4$	$(3.6704*10^{21})\ e^{-287756.8/(8.314T)}\ P_{C6H12}$
$4.5C_{10}H_{22} + 4.5H_2 \rightarrow C_9H_{20} + C_8H_{18} + C_7H_{16} + C_6H_{14} + C_5H_{12} + C_4H_{10} + C_3H_8 + C_2H_6 + CH_4$	$(3.6704*10^{21})\ e^{-287756.8/(8.314T)}\ P_{C10H22}$
$C_6H_{12} + H_2 \rightarrow C_6H_{14}$	$(3.33674*10^{19})\ e^{-275285.8/(8.314T)}\ P_{C6H12}P_{H2} - (4.19816*10^{21})e^{-312237.9/(8.314T)}P_{C6H12}$

Vapors leaving V-101 are split with 5% being purged (stream 15) and the rest being sent back as recycle (stream 12) to be compressed in K-101 and combined with the unheated feed (stream 2) after it has been pumped from P-101. Liquid leaving V-101 is cooled in E-103 and fed (stream 18) into T-101 at the top stage. T-101 has no condenser and overhead vapors (stream 19) are used as a smaller hydrocarbon product stream for no economic benefit to the plant leaving at 198.8^{o}F and 90 psia. T-101 is designed with 25 stages operating at 80% efficiency. The partial reboiler (E-104) that uses 150 psig steam connected to T-101 has a boilup ratio of 0.5528 and the bottoms product leaving T-101 is then cooled in E-105 and used as feed (stream 24) into the bottom of the first extractor (LLE-101) at 150^{o}F and 45 psia. Sulfolane is fed (stream 31) at

252.3°F and 15 psia into the top of LLE-101 which has 20 stages. The bottoms product leaving the extractor (stream 32), which is primarily benzene and sulfolane, is fed into the top stage of T-102. The overhead product leaving the first extractor (stream 25) is then fed into the bottom of the second extractor (LLE-102) that has 30 stages and a top feed (stream 27) of water at 72°F and 75 psia. Hydrocarbons ranging from n-pentane to n-decane are the primary product leaving the top of the second extractor (stream 28) at 236.5°F and 30 psia while the bottoms product (stream 26) are purged and treated as a waste product. T-102 has no condenser, yet it has a partial reboiler (E-108) using 450 psig steam and 7 stages operating at 80% efficiency. The bottoms product (stream 37), which is mainly sulfolane, is recylcled back and mixed with the feed sulfolane (stream 29) to be used as the top feed (stream 31) into LLE-101 mentioned above. The overhead vapor product from T-102 (stream 33) is cooled (E-107) with cooling water at 25°C and fed (stream 35) into T-103 at stage 8 of 23 counting from top to bottom. T-103 has a partial reboiler (E-110) using 150 psig steam and total condenser (E-109). The distillate (stream 46) is mixed with stream 22 to form stream 23 to be cooled in E-105 and used as feed (stream 24) into the bottom of the first extractor (LLE-101) mentioned above. The bottoms product (stream 49) is mainly benzene which is cooled and fed into T-104 at stage 9 of 20. The total condenser (E-111) in T-104 has a reflux ratio of 0.6, and the partial reboiler (E-112) using 150 psig steam has a boil-up ratio of 3.062. The distillate is a benzene product at 99% purity (stream 55) at 182.5°F and 15 psia with toluene and para-xylene leaving as bottoms product to be fed (stream 58) into T-105 which has 43 trays operating at 80% efficiency with the feed at stage 15. This final column has a reflux ratio and boil-up ratio of 3.557 and 3.277 for the total condenser (E-113) and a partial reboiler (E-114) using 450 psig steam respectively. The distillate is the toluene product (stream 64) at 232.4°F and 15 psia with the bottoms being the para-xylene product (stream 67) at 383°F and 53 psia. Both streams are at 99% purity. The Process Flow Diagrams (PFDs) below give further guidance to the operation of our process in Figures 1-3 with stream tables given as well in Table 3.

Process Flow Diagram

PFDs which highlight the process topology, stream information, and equipment information for the process are given below. Figure 1 highlights the reactor section of the process; Figure 2 highlights the extraction section of the process, and Figure 3 highlights the distillation section of the process. Stream tables, describing many of the key streams in the process and outlining major mass balances, are shown below in Table 3. Furthermore, key parameters regarding the equipment used to design the plant are given in Table 4, which is modeled for the Feed K.

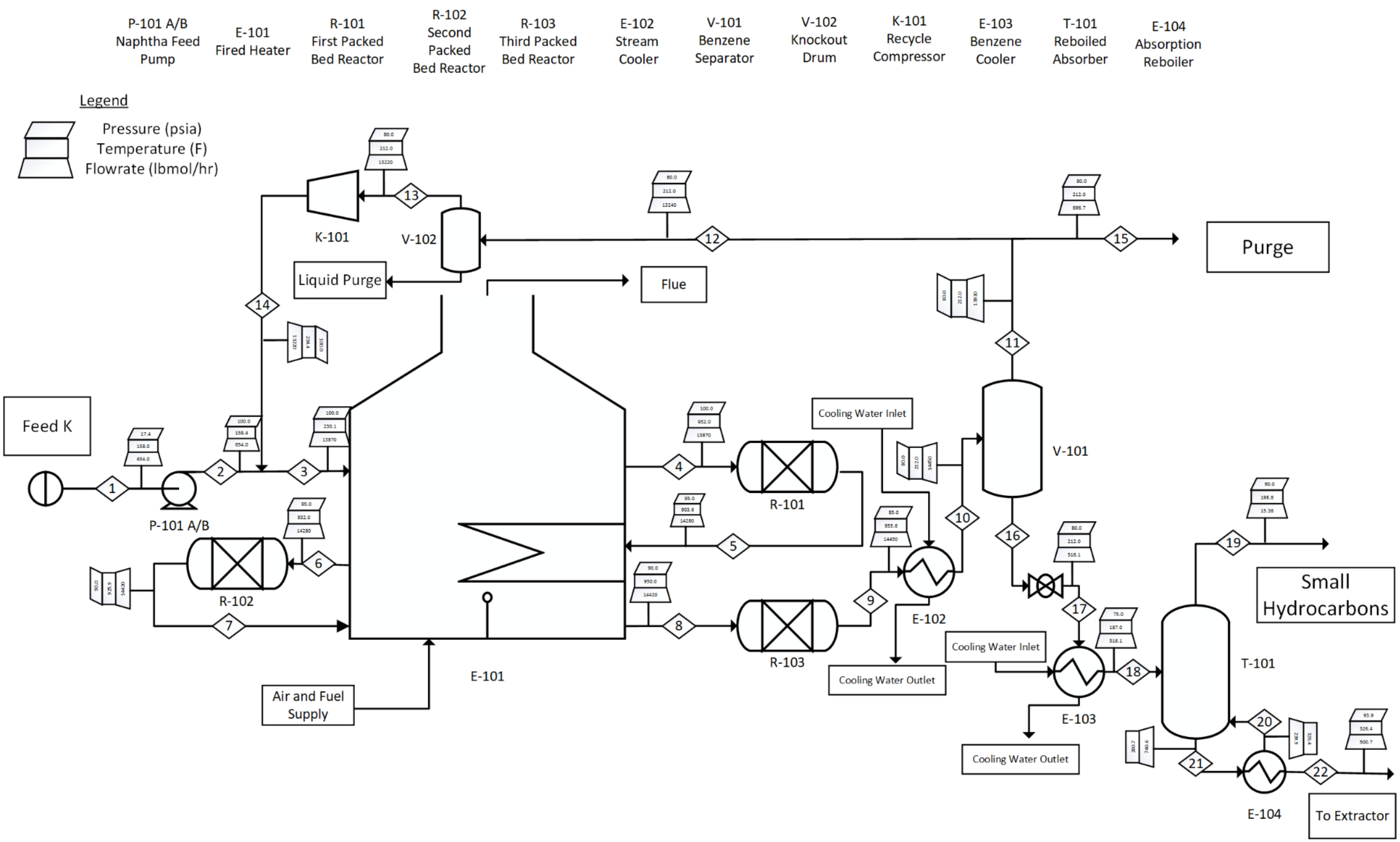


Figure 1: Reactor Section PFD

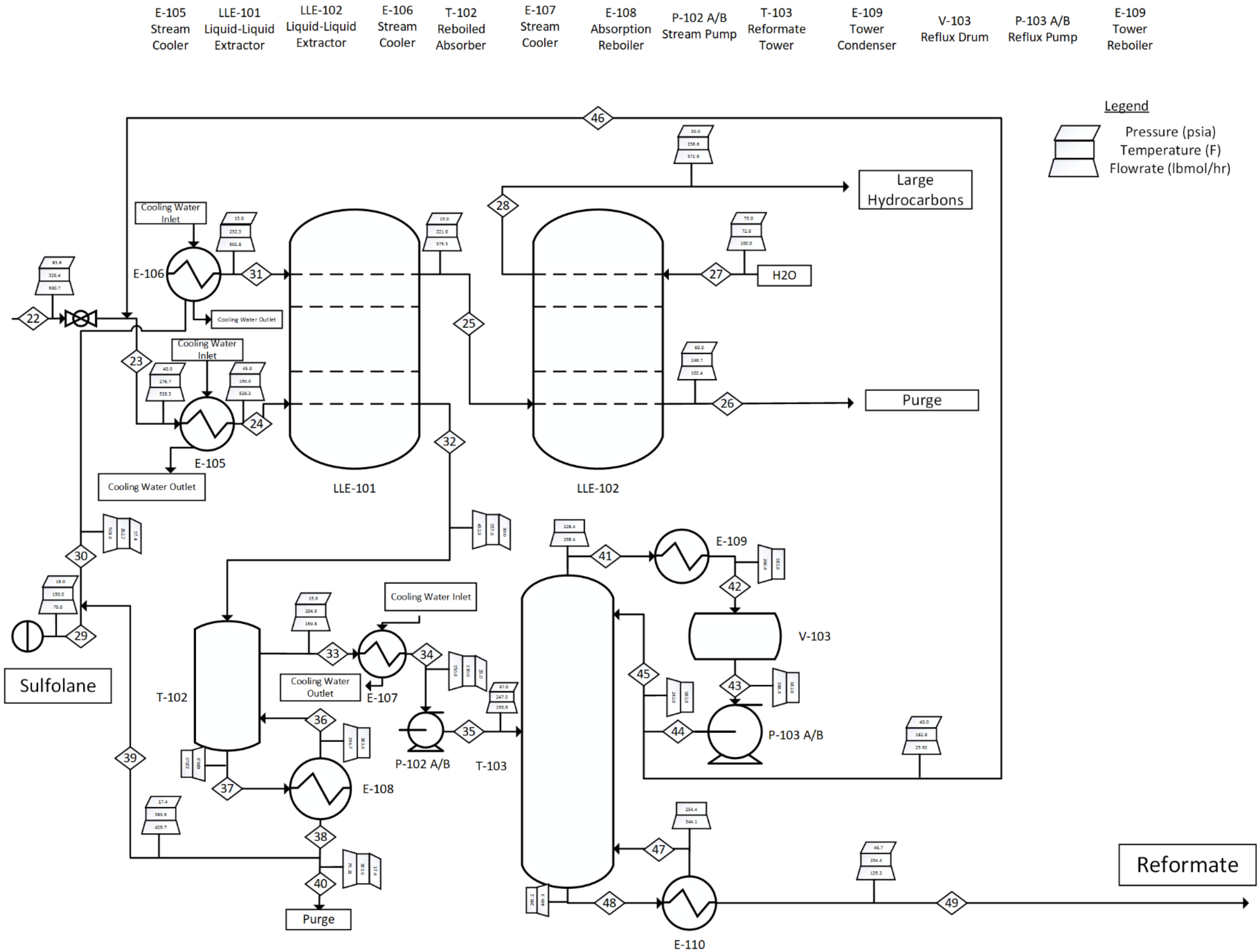


Figure 2: Extraction Section PFD

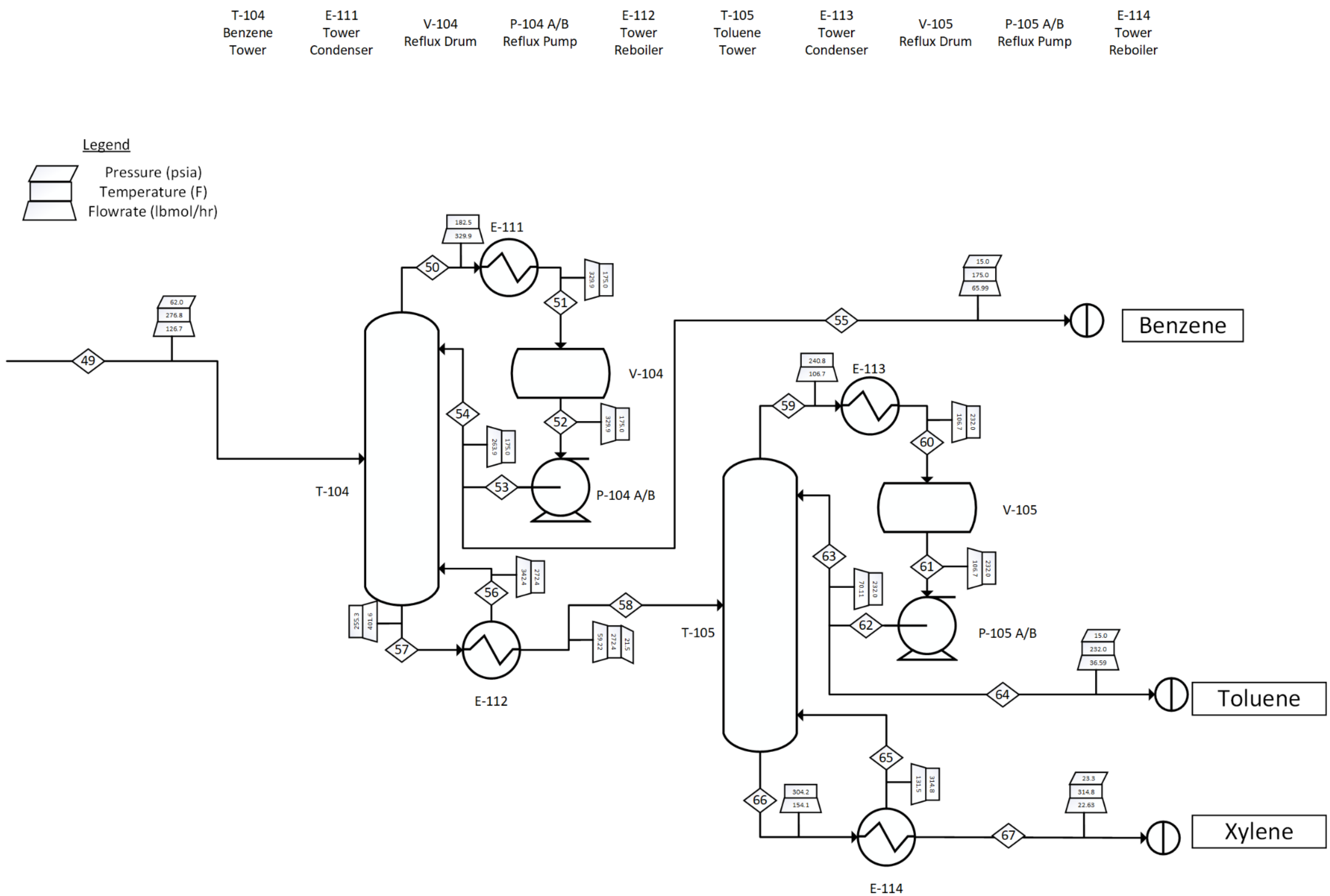


Figure 3: Distillation Section PFD

Table 3: Stream Tables for Feed K

Stream Number	Feed K (1)	2	3	4	5	6	7	8	9	10	11
Phase Fraction	0.0	0.0	0.9378	1.0	1.0	1.0	1.0	1.0	1.0	0.9643	1.0
Temperature (F)	158.0	158.43	230.15	932.0	903.61	932.0	925.9	950.0	955.59	212.0	212.0
Pressure (psia)	17.4045	100.0	100.0	100.0	95.0	95.0	90.0	90.0	85.0	80.0	80.0
Molar Enthalpy (Btu/lbmole)	-9.08E+04	-9.08E+04	-1.91E+04	-5.06E+02	-4.91E+02	3.36E+02	3.33E+02	1.03E+03	1.03E+03	-1.75E+04	-1.59E+04
Mass flow rate (lb/hr)	7.74E+04	7.74E+04	5.17E+05	5.17E+05	5.17E+05	5.17E+05	5.17E+05	5.17E+05	5.17E+05	5.17E+05	4.64E+05
Molar flow rate (lbmol/hr)	6.54E+02	6.54E+02	1.39E+04	1.39E+04	1.43E+04	1.43E+04	1.44E+04	1.44E+04	1.45E+04	1.45E+04	1.39E+04
Volumetric Flow rate	1.74E+03	1.74E+03	9.40E+05	2.07E+06	2.20E+06	2.24E+06	2.38E+06	2.42E+06	2.58E+06	1.23E+06	1.23E+06
Actual Density (lb/ft.^3)	44.36	44.39	0.55	0.25	0.24	0.23	0.22	0.21	0.2	0.42	0.38
Std Ideal Liq Vol Flow(barrel/day)	7.06E+03	7.06E+03	6.67E+04	6.67E+04	6.74E+04	6.74E+04	6.77E+04	6.77E+04	6.79E+04	6.79E+04	6.29E+04
Comp Mole Frac (n-Pentane)	---	---	0.052	0.052	0.0514	0.0514	0.0523	0.0523	0.0544	0.0544	0.0545
Comp Mole Frac (n-Hexane)	---	---	0.0258	0.0258	0.0257	0.0257	0.0265	0.0265	0.0282	0.0282	0.0272
Comp Mole Frac (n-Heptane)	---	---	0.0177	0.0177	0.0178	0.0178	0.0188	0.0188	0.021	0.021	0.0186
Comp Mole Frac (n-Octane)	---	---	0.0093	0.0093	0.0097	0.0097	0.0108	0.0108	0.013	0.013	0.0098
Comp Mole Frac (n-Nonane)	---	---	0.0048	0.0048	0.0053	0.0053	0.0065	0.0065	0.0087	0.0087	0.005
Comp Mole Frac (n-Decane)	0.597	0.597	0.0335	0.0335	0.0296	0.0296	0.024	0.024	0.0139	0.0139	0.0056
Comp Mole Frac (Methane)	---	---	0.0877	0.0877	0.0861	0.0861	0.0866	0.0866	0.0887	0.0887	0.0919
Comp Mole Frac (Ethane)	---	---	0.0844	0.0844	0.083	0.083	0.0835	0.0835	0.0855	0.0855	0.0885
Comp Mole Frac (Propane)	---	---	0.0785	0.0785	0.0772	0.0772	0.0778	0.0778	0.0798	0.0798	0.0823
Comp Mole Frac (n-Butane)	---	---	0.0659	0.0659	0.065	0.065	0.0656	0.0656	0.0677	0.0677	0.0692
Comp Mole Frac (Hydrogen)	---	---	0.4	0.4	0.4135	0.4135	0.4135	0.4135	0.4048	0.4048	0.4197
Comp Mole Frac (Benzene)	0.09	0.09	0.1256	0.1256	0.1318	0.1318	0.1338	0.1338	0.1341	0.1341	0.1277
Comp Mole Frac (Cyclohexane)	0.313	0.313	0.0148	0.0148	0.0039	0.0039	0.0005	0.0005	0.0001	0.0001	0.0001

Stream Number	12	13	14	15	16	17	18	19	20	21	22
Phase Fraction	1.0	1.0	1.0	1.0	0.0	0.0003	0.0	1.0	1.0	0.0	0.0
Temperature (F)	212.0	212.0	234.42	212.0	212.0	212.0	187.0	198.84	326.43	280.75	326.43
Pressure (psia)	80.0	80.0	100.0	80.0	80.0	80.0	75.0	90.0	93.9	91.9	93.9
Molar Enthalpy (Btu/lbmole)	-1.59E+04	-1.59E+04	-1.55E+04	-1.59E+04	-5.99E+04	-6.00E+04	-6.15E+04	-3.33E+04	-2.01E+04	-4.86E+04	-5.33E+04
Mass flow rate (lb/hr)	4.41E+05	4.40E+05	4.40E+05	2.32E+04	5.31E+04	5.31E+04	5.31E+04	6.65E+02	1.91E+04	7.16E+04	5.25E+04
Molar flow rate (lbmol/hr)	1.32E+04	1.32E+04	1.32E+04	6.97E+02	5.16E+02	5.16E+02	5.16E+02	1.54E+01	2.40E+02	7.41E+02	5.01E+02
Volumetric Flow rate	1.16E+06	1.16E+06	9.59E+05	6.13E+04	1.27E+03	1.28E+03	1.24E+03	1.21E+03	2.16E+04	1.84E+03	1.39E+03
Actual Density (lb/ft.^3)	0.38	0.38	0.46	0.38	41.89	41.48	42.76	0.55	0.89	38.94	37.84
Std Ideal Liq Vol Flow(barrel/day)	5.98E+04	5.97E+04	5.97E+04	3.15E+03	4.93E+03	4.93E+03	4.93E+03	8.89E+01	1.82E+03	6.66E+03	4.84E+03
Comp Mole Frac (n-Pentane)	0.0545	0.0545	0.0545	0.0545	0.05	0.05	0.05	0.0436	0.1719	0.0669	0.0502
Comp Mole Frac (n-Hexane)	0.0271	0.0271	0.0271	0.0272	0.0574	0.0574	0.0574	0.0175	0.0895	0.0612	0.0586
Comp Mole Frac (n-Heptane)	0.0186	0.0186	0.0186	0.0186	0.0875	0.0875	0.0875	0.0106	0.069	0.0861	0.0898
Comp Mole Frac (n-Octane)	0.0098	0.0098	0.0098	0.0098	0.0993	0.0993	0.0993	0.0052	0.0415	0.0975	0.1022
Comp Mole Frac (n-Nonane)	0.005	0.005	0.005	0.005	0.1063	0.1063	0.1063	0.0024	0.0237	0.1084	0.1095
Comp Mole Frac (n-Decane)	0.0056	0.0056	0.0056	0.0056	0.2402	0.2402	0.2402	0.002	0.0251	0.2583	0.2476
Comp Mole Frac (Methane)	0.092	0.092	0.092	0.0919	0.0018	0.0018	0.0018	0.0615	---	---	---
Comp Mole Frac (Ethane)	0.0886	0.0886	0.0886	0.0885	0.0059	0.0059	0.0059	0.1975	---	---	---
Comp Mole Frac (Propane)	0.0824	0.0824	0.0824	0.0823	0.0133	0.0133	0.0133	0.4401	0.0047	0.0008	0.0002
Comp Mole Frac (n-Butane)	0.0691	0.0691	0.0691	0.0692	0.0282	0.0282	0.0282	0.0683	0.1883	0.0476	0.0269
Comp Mole Frac (Hydrogen)	0.4198	0.4198	0.4198	0.4197	0.0023	0.0023	0.0023	0.0757	---	---	---
Comp Mole Frac (Benzene)	0.1274	0.1274	0.1274	0.1277	0.3076	0.3076	0.3076	0.0755	0.386	0.273	0.3148
Comp Mole Frac (Cyclohexane)	0.0001	0.0001	0.0001	0.0001	0.0003	0.0003	0.0003	0.0001	0.0003	0.0002	0.0003

Stream Number	23	24	25	26	27	28	Sulfolane (29)	30	31	32	33	34	35
Phase Fraction	0.2579	0.0	0.1656	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Temperature (F)	276.74	150.0	220.99	248.73	72.0	236.57	150.0	352.77	252.3	157.62	204.94	130.0	130.0
Pressure (psia)	40.0	45.0	15.0	60.0	75.0	30.0	18.0	17.4	15.0	30.0	15.0	25.0	25.0
Molar Enthalpy (Btu/lbmole)	-5.07E+04	-6.12E+04	-8.83E+04	-1.22E+05	-1.23E+05	-8.79E+04	-1.92E+05	-1.73E+05	-1.79E+05	-1.36E+05	3.34E+04	1.81E+04	1.81E+04
Mass flow rate (lb/hr)	5.44E+04	5.44E+04	4.27E+04	2.21E+03	1.80E+03	4.23E+04	9.01E+03	5.97E+04	5.97E+04	7.14E+04	1.17E+04	1.17E+04	1.17E+04
Molar flow rate (lbmol/hr)	526.34	526.34	375.25	102.4	100.0	372.85	75.0	501.75	501.75	652.84	150.82	150.82	150.82
Volumetric Flow rate	2.79E+04	1.23E+03	3.12E+04	3.76E+01	2.86E+01	4.72E+03	1.18E+02	5.18E+03	8.35E+02	1.03E+03	7.17E+04	2.28E+02	2.28E+02
Actual Density (lb/ft.^3)	1.95	44.36	1.37	58.64	63.02	8.98	76.19	11.54	71.56	69.54	0.16	51.57	51.57
Std Ideal Liq Vol Flow(barrel/day)	5.01E+03	5.01E+03	4.07E+03	1.45E+02	1.24E+02	4.05E+03	4.87E+02	3.30E+03	3.30E+03	4.23E+03	9.28E+02	9.28E+02	9.28E+02
Comp Mole Frac (n-Pentane)	0.0534	0.0534	0.067	---	---	0.0674	---	---	---	0.0046	0.0198	0.0198	0.0198
Comp Mole Frac (n-Hexane)	0.0582	0.0582	0.0778	---	---	0.0783	---	0.0016	0.0016	0.0035	0.0088	0.0088	0.0088
Comp Mole Frac (n-Heptane)	0.0855	0.0855	0.1181	---	---	0.1188	---	0.0034	0.0034	0.0037	0.0027	0.0027	0.0027
Comp Mole Frac (n-Octane)	0.0972	0.0972	0.1352	---	---	0.1361	---	0.0032	0.0032	0.0031	0.0009	0.0009	0.0009
Comp Mole Frac (n-Nonane)	0.1041	0.1041	0.1449	---	---	0.1459	---	0.0041	0.0041	0.0038	0.0004	0.0004	0.0004
Comp Mole Frac (n-Decane)	0.2355	0.2355	0.3291	---	---	0.3312	---	0.0049	0.0049	0.0044	0.0002	0.0002	0.0002
Comp Mole Frac (Propane)	0.0004	0.0004	0.0004	---	---	0.0004	---	---	---	---	0.0003	0.0003	0.0003
Comp Mole Frac (n-Butane)	0.0305	0.0305	0.0359	0.0001	---	0.0361	---	---	---	0.0039	0.0169	0.0169	0.0169
Comp Mole Frac (Benzene)	0.3349	0.3349	0.082	0.0003	---	0.0824	---	0.0269	0.0269	0.2436	0.949	0.949	0.949
Comp Mole Frac (Cyclohexane)	0.0002	0.0002	0.0003	---	---	0.0003	---	---	---	---	---	---	---
Comp Mole Frac (H2O)	---	---	---	0.9652	1.0	0.0031	---	---	---	---	---	---	---
Comp Mole Frac (SULFOLANE)	---	---	0.0093	0.0342	---	---	1.0	0.9559	0.9559	0.7293	0.0009	0.0009	0.0009

Stream Number	36	37	38	39	40	41	42	43	44	45	46	47
Phase Fraction	1.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0
Temperature (F)	383.61	219.96	383.61	383.61	383.61	228.38	182.81	182.81	182.81	182.81	182.81	254.39
Pressure (psia)	17.4	15.4	17.4	17.4	17.4	42.0	40.0	40.0	40.0	40.0	40.0	46.7
Molar Enthalpy (Btu/lbmole)	1.93E+04	-1.29E+05	-1.70E+05	-1.70E+05	-1.70E+05	1.29E+04	-1.96E+02	-1.96E+02	-1.96E+02	-1.96E+02	-2.78E+02	3.91E+04
Mass flow rate (lb/hr)	1.64E+04	7.61E+04	5.97E+04	5.07E+04	8.95E+03	2.13E+04	1.94E+04	1.94E+04	1.94E+04	1.94E+04	1.94E+03	2.69E+04
Molar flow rate (lbmol/hr)	196.75	698.77	502.02	426.72	75.3	281.7	256.09	256.09	256.09	256.09	25.61	343.85
Volumetric Flow rate	1.02E+05	1.14E+03	8.89E+02	7.56E+02	1.33E+02	4.62E+04	4.26E+02	4.26E+02	4.26E+02	4.26E+02	4.26E+01	5.24E+04
Actual Density (lb/ft.^3)	0.16	66.53	67.07	67.07	67.07	0.46	45.57	45.57	45.57	45.57	45.57	0.51
Std Ideal Liq Vol Flow(barrel/day)	1.28E+03	4.58E+03	3.30E+03	2.81E+03	4.96E+02	1.83E+03	1.66E+03	1.66E+03	1.66E+03	1.66E+03	1.66E+02	2.09E+03
Comp Mole Frac (n-Pentane)	0.0013	0.0004	---	---	---	0.1166	0.1166	0.1166	0.1166	0.1166	0.1166	---
Comp Mole Frac (n-Hexane)	0.0258	0.0086	0.0019	0.0019	0.0019	0.0515	0.0515	0.0515	0.0515	0.0515	0.0515	---
Comp Mole Frac (n-Heptane)	0.0295	0.0112	0.004	0.004	0.004	0.0008	0.0008	0.0008	0.0008	0.0008	0.0008	0.0027
Comp Mole Frac (n-Octane)	0.0155	0.007	0.0037	0.0037	0.0037	---	---	---	---	---	---	0.0005
Comp Mole Frac (n-Nonane)	0.0113	0.0066	0.0048	0.0048	0.0048	---	---	---	---	---	---	0.0002
Comp Mole Frac (n-Decane)	0.0072	0.0061	0.0057	0.0057	0.0057	---	---	---	---	---	---	---
Comp Mole Frac (Propane)	---	---	---	---	---	0.002	0.002	0.002	0.002	0.002	0.002	---
Comp Mole Frac (n-Butane)	---	---	---	---	---	0.0998	0.0998	0.0998	0.0998	0.0998	0.0998	---
Comp Mole Frac (Benzene)	0.8366	0.2583	0.0317	0.0317	0.0317	0.7293	0.7293	0.7293	0.7293	0.7293	0.7293	0.9964
Comp Mole Frac (SULFOLANE)	0.0725	0.7016	0.9482	0.9482	0.9482	---	---	---	---	---	---	---

Stream Number	48	49	50	51	52	53	54	Benzene (55)	56	57
Phase Fraction	0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0
Temperature (F)	249.24	254.39	182.47	175.0	175.0	175.0	175.0	175.0	272.43	255.28
Pressure (psia)	43.7	46.7	17.0	15.0	15.0	15.0	15.0	15.0	21.5	18.5
Molar Enthalpy (Btu/lbmole)	2.66E+04	1.71E+04	3.73E+04	2.39E+04	2.39E+04	2.39E+04	2.39E+04	2.39E+04	2.42E+04	8.77E+03
Mass flow rate (lb/hr)	3.67E+04	1.09E+04	3.10E+04	2.58E+04	2.58E+04	2.58E+04	2.58E+04	5.16E+03	3.26E+04	3.84E+04
Molar flow rate (lbmol/hr)	4.69E+02	1.25E+02	3.96E+02	3.30E+02	3.30E+02	3.30E+02	3.30E+02	6.60E+01	3.42E+02	4.02E+02
Volumetric Flow rate	7.72E+02	2.29E+02	1.61E+05	5.10E+02	5.10E+02	5.10E+02	5.10E+02	1.02E+02	1.25E+05	8.02E+02
Actual Density (lb/ft.^3)	47.53	47.78	0.19	50.58	50.58	50.58	50.58	50.58	0.26	47.82
Std Ideal Liq Vol Flow(barrel/day)	2.85E+03	8.58E+02	2.41E+03	2.01E+03	2.01E+03	2.01E+03	2.01E+03	4.02E+02	2.57E+03	3.03E+03
Comp Mole Frac (n-Heptane)	0.0028	0.0031	0.0056	0.0056	0.0056	0.0056	0.0056	0.0056	0.0006	0.0005
Comp Mole Frac (n-Octane)	0.0007	0.001	---	---	---	---	---	---	0.0024	0.0024
Comp Mole Frac (n-Nonane)	0.0002	0.0005	---	---	---	---	---	---	0.0005	0.0006
Comp Mole Frac (n-Decane)	---	0.0002	---	---	---	---	---	---	0.0001	0.0002
Comp Mole Frac (Benzene)	0.9958	0.5252	0.9936	0.9936	0.9936	0.9936	0.9936	0.9936	0.0091	0.0082
Comp Mole Frac (Toluene)	---	0.2897	0.0007	0.0007	0.0007	0.0007	0.0007	0.0007	0.7647	0.7422
Comp Mole Frac (p-Xylene)	---	0.1791	---	---	---	---	---	---	0.2226	0.2456

Stream Number	58	59	60	61	62	63	Toluene (64)	65	66	Xylenes (67)
Phase Fraction	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Temperature (F)	272.43	240.41	232.02	232.02	232.02	232.02	232.02	314.82	304.19	314.81
Pressure (psia)	21.5	17.0	15.0	15.0	15.0	15.0	15.0	23.3	20.3	23.3
Molar Enthalpy (Btu/lbmole)	7.16E+03	2.58E+04	1.13E+04	1.13E+04	1.13E+04	1.13E+04	1.13E+04	1.61E+04	3.00E+02	-1.41E+02
Mass flow rate (lb/hr)	5.78E+03	1.31E+04	9.70E+03	9.70E+03	9.70E+03	9.70E+03	3.37E+03	1.38E+04	1.62E+04	2.41E+03
Molar flow rate (lbmol/hr)	59.22	141.83	105.24	105.24	105.24	105.24	36.59	130.15	152.78	22.63
Volumetric Flow rate	1.22E+02	6.27E+04	1.99E+02	1.99E+02	1.99E+02	1.99E+02	6.93E+01	4.64E+04	3.52E+02	5.28E+01
Actual Density (lb/ft.^3)	47.25	0.21	48.65	48.65	48.65	48.65	48.65	0.3	46.14	45.62
Std Ideal Liq Vol Flow(barrel/day)	4.56E+02	1.03E+03	7.64E+02	7.64E+02	7.64E+02	7.64E+02	2.66E+02	1.10E+03	1.29E+03	1.90E+02
Comp Mole Frac (n-Heptane)	0.0003	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004	---	---	---
Comp Mole Frac (n-Octane)	0.0022	0.0036	0.0036	0.0036	0.0036	0.0036	0.0036	---	---	---
Comp Mole Frac (n-Nonane)	0.0011	---	---	---	---	---	---	0.0026	0.0023	0.0029
Comp Mole Frac (n-Decane)	0.0005	---	---	---	---	---	---	0.0007	0.0006	0.0013
Comp Mole Frac (Toluene)	0.6118	0.99	0.99	0.99	0.99	0.99	0.99	---	---	---
Comp Mole Frac (p-Xylene)	0.3786	0.0006	0.0006	0.0006	0.0006	0.0006	0.0006	0.9965	0.9961	0.99

Table 4: Equipment Tables for Feed K

Heat Exchangers	E-102	E-103	E-104	E-105	E-106	E-107	E-108	E-109	E-110	E-111	E-112	E-113	E-114
Type	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head	Floating Head
Area(ft^2)	3620	37.12	377.2	267.7	74.95	187.2	248.9	178.2	222.5	331.0	167.0	75.16	179.6
Duty(Btu/hr)	2.671E+08	7.519E+05	4.496E+06	5.515E+06	3.002E+06	2.319E+06	8.524E+06	3.697E+06	5.182E+06	5.319E+06	1.760E+06	2.083E+06	2.069E+06
Shell													
Temp(F)	77	77	355.82	77	77	77	453.02	77	355.82	77	355.82	77	355.82
Pres. (psia)	14.7	14.7	135	14.7	14.7	14.7	435	14.7	135	14.7	135	14.7	135
Phase	0	0	1	0	0	0	1	0	1	0	1	0	1
MOC	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.
Tube													
Temp(F)	955.6	212	280.7	276.7	352.8	204.9	220	228.4	255.3	182.5	305.9	204.4	304.2
Pres. (psig)	85	80	91.9	40	17.4	15	17.4	42	43.7	17	18.5	17	20.3
Phase	1	0	0	0.2579	0.0172	1	0	1	0	1	0	1	0
MOC	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.

Vessels/Towers	T-101	T-102	T-103	T-104	T-105	V-101	V-102	V-103	V-104	V-105	LLE-101	LLE-102
Temperature(F)	280	228.1	248.9	255	303.9	212	212	182.8	175	232	250	250
Pres. (psia)	91.9	15.4	43.7	18.5	20.3	80	80	40	15	15	30	
Orientation	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical	Vertical	Horizontal	Horizontal	Horizontal	Vertical	Vertical
MOC	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.	S.S.
Size												
Height/Length (ft.)	60	24	56	50	96	7.189	7.053	4.675	2.5	2	60	86
Diameter (ft.)	7	9	9.5	13.5	9	2.167	2.053	2.5	3.894	3.66	4.91	3.43
Internals	20 C.S. Sieve Trays	5 C.S Sieve Trays	18 C.S. Sieve Trays	16 C.S. Sieve Trays	34 C.S Sieve Trays	---	---	---	---	---	20 C.S. Sieve Trays	30 S.S. Sieve Trays

Pumps/Compressors	P-101A/B	P-102A/B	P-103A/B	P-104A/B	P-105A/B	C-101
Flow (lb/hr)	77382	11007	10876	4327	5237	439883
Fluid Density (lb/ft^3)	44.36	50.47	43.44	50.30	48.62	0.3782
Power (hp)	14.73	1.57	1.5	0.5	0.94	1910
Pressure in (psi)	17	24.8	42.5	18	17.9	80
Pressure out (psi)	133	114.6	117.5	90	127	100
Temperature (F)	158	130	182.8	175	232	212
Efficiency	0.5	0.5	0.5	0.5	0.5	0.8
Type/Drive	Centrifugal/Electric	Centrifugal/Electric	Centrifugal/Electric	Centrifugal/Electric	Centrifugal/Electric	Centrifugal/Electric
MOC	C.S.	C.S.	C.S.	C.S.	C.S.	C.S.

Reactors	R-101	R-102	R-103
Temperature (F)	932	932	950
Pres. (psia)	100	95	90
Orientation	Horizontal	Horizontal	Horizontal
MOC	C.S	C.S	C.S
Size			
Length (ft)	16.41	18.04	21.33
Diameter (ft)	8.202	9.514	9.843
Volume (ft^3)	867.1	1283	1623
Catalyst			
Particle Diameter (ft)	5.25E-03	5.25E-03	5.25E-03
Particle Sphericity	1	1	1
Solid Density (lb/ft^3)	46.20	46.20	46.20
Bulk Density (lb/ft^3)	23.10	23.10	23.10
Solid Heat Capacity (Btu/lb-F)	3.48E-02	3.48E-02	3.48E-02

Economic Analysis and Sensitivities

Capital Cost Estimates

This report provides capital cost estimates on the basis of being incurred in the 2021 budget. The estimates provided can be assumed to be accurate within a ± 20% range of the true capital cost [1]. A detailed design could determine more accurate estimates should the project be chosen to proceed. Our team employed a modified Guthrie method to determine capital cost estimates [2]. This method is based on numerous factors including a capacity factor, design pressure, and materials of construction, MOC. The equations below allowed our team to calculate free on board purchased and bare module cost, respectively, in the year 2001. Installed costs take MOC and pressure factors into account. Constants for each piece of equipment vary and can be found in literature [1].

$$\text{Log } C_p^0 = k_1 + k_2 \log[A] + k_3 \log^2[A] \qquad \text{(Eq. 1)}$$

$$C_{BM} = C_p^0 (B_1 + B_2 F_m F_p) \qquad \text{(Eq. 2)}$$

The project team escalated costs calculated for the year 2001 to present day using the 2020 mid-year Chemical Engineering Plant Cost Index, CEPCI [3]. The cost index provided values ranging back to the mid 1990s to as recent as nearly present day. While the current CEPCI was unavailable to our team, one could assume the value would be slightly larger (within 20 points) based on recent trends in the index. This was a potential source for inaccuracy since capital costs are accounted for in 2021, which is why all costing was done conservatively in this report to counteract any under-costing such inaccuracies would cause. The CEPCI for 2001 is 397 while the 2020 value is 594. Calculated capital costs factor in: MOC, maximum allowable operating pressure (MAWP), installation, infrastructure, and contingency and fees associated with the process.

In order to calculate the MAWP, 50 psi or 10% of the total pressure for the vessel was added to design pressures, whichever was larger. This safety factor allows for pressure spikes to occur without affecting the mechanical integrity of the equipment. Equipment, such as pumps, is oversized in these calculations for similar reasons. As instructed in the project memorandum, the team sized feed K and feed TQ1 separately. In order to ensure both streams could run through the same facility, the larger equipment of the two streams, and thus the more expensive equipment, was used for capital cost calculations. Capital costs associated for the equipment used in this process are listed below in Table 5. The fired heater (E-101) takes up the largest portion of the capital cost. The heat generated in this piece of equipment is crucial for the effectiveness of the reactions in R-101-103. Extractors and distillation columns take up the next largest chunk of cost with pumps and separators taking up the smallest portion.

Table 5: Capital Costs

Capital Costs: Feed K & TQ1			
Equipment	Cost	Equipment	Cost
R - 101	$389,000	E - 104	$94,200
R - 102	$450,000	E - 105	$92,800
R - 103	$487,000	E - 106	$108,000
V -101	$10,700	E - 107	$105,000
V -102	$9,970	E - 108	$111,000
V -103	$8,500	E - 109	$91,600
V -104	$142,000	E - 110	$93,300
V -105	$148,000	E - 111	$96,900
T - 101	$492,000	E - 112	$116,000
T - 102	$317,000	E - 113	$182,000
T - 103	$781,000	E - 114	$118,000
T - 104	$1,390,000	P - 101 A/B	$33,700
T - 105	$917,000	P - 102 A/B	$14,500
LLE -101	$2,040,000	P - 103 A/B	$14,500
LLE -102	$1,950,000	P - 104 A/B	$11,900
E - 101	$138,000,000	P - 105 A/B	$12,300
E - 102	$278,000	K - 101	$1,750,000
E - 103	$145,000	**Total**	**$151,000,000**

Revenue Estimates

The project team determined the revenues associated with feed streams K and TQ1 separately leading to two different branches of economic analysis. Calculations done on a yearly basis have a service factor of 0.92. There are 4 separate streams with 5 different products producing revenue. The final two columns in our process, T-104 and T-105, produced benzene, toluene, and xylene as mentioned above. The second extractor's overhead product stream produced linear alkanes. Gasoline product sales include cyclic hydrocarbons and chained hydrocarbons ranging from n-pentane to n-octane. Diesel product sales include chained hydrocarbons ranging from n-nonane and up. Prices associated with sales are given below in Table 6. This table also depicts the flow rate and revenue produced for each stream for feed K. Table 7 lists the revenues from feed TQ1. Diesel sales for both feeds account for the largest revenue source. Toluene takes up the smallest portion for each feed. Overall TQ1 produces more revenue than K.

Table 6: Feed K Revenue Streams

Product Stream	Price	Flow Rate (lb/hr)	Yearly Income
Benzene	$3.49/gal	5160	$23,500,000
Toluene	$2.792/gal	3370	$12,700,000
Xylene	$2.792/gal	2410	$10,300,000
Diesel	$0.98/L	20200	$538,000,000
Gasoline	$0.63/L	17000	$291,000,000
Total			$876,000,000

Table 7: Feed TQ1 Revenue Streams

Product Stream	Price	Flow Rate (lb/hr)	Yearly Income
Benzene	$3.49/gal	1300	$5,930,000
Toluene	$2.792/gal	1580	$5,950,000
Xylene	$2.792/gal	1120	$4,800,000
Diesel	$0.98/L	29200	$778,000,000
Gasoline	$0.63/L	30600	$523,000,000
Total			$1,320,000,000

Operating Expense Estimates

Operating costs include raw materials, waste treatment, utilities, and operating labor. Raw materials generally account for the greatest portion of operating costs [1]. Naphtha and sulfolane cost $0.325/L and $5/kg, respectively. Literature provided costs for process water [1]. For stream K, the sulfolane feed stream was the greatest raw material cost. Stream TQ1 differed in this component with a much higher naphtha feed stream cost compared to K making its naphtha stream cost greater than that of sulfolane. Process water costs were so low they are negligible in comparison. Tables 8 and 9 depict these costs below. Overall TQ1 has a greater raw material cost than K.

Table 8: Feed K Raw Material Costs

Feed Streams	Flow Rate (lb/hr)	Yearly Cost
Naphtha	77,400	$133,000,000
Sulfolane	9,010	$179,000,000
Water	1,800	$1,270
Total		$312,000,000

Table 9: Feed TQ1 Raw Material Costs

Feed Streams	Flow Rate (lb/hr)	Yearly Cost
Naphtha	106,000	$184,000,000
Sulfolane	9,010	$179,000,000
Water	1,800	$1,270
		$363,000,000

This project is considered revenue producing as opposed to service producing. Waste treatment handles hazardous and non-hazardous product streams in this process that are not gaining revenue. These waste products, if not handled appropriately, could have adverse effects on people and the environment. Waste in this process is seen through the three purge streams: streams 15, 26, and 39. Costs associated with treating our waste are derived from literature [1].

Waste stream costs are seen below for each stream in Tables 10 and 11. Stream 15 incurs the most yearly cost with stream 39 incurring the least yearly cost for both feed streams.

Table 10: Feed K Waste Costs

Stream #	Flow Rate (lb/hr)	Yearly Cost
15	23200	$3,050,000
26	2210	$290,000
39	8950	$1,180,000

Table 11: Feed TQ1 Waste Costs

Stream #	Flow Rate (lb/hr)	Yearly Cost
15	24500	$3,220,000
26	2570	$338,000
39	8400	$1,100,000

A successful process with this much equipment requires operators. The equation below estimated the required number of operators needed per shift with P representing particulate solid process steps and N_{np} representing the total pieces of equipment.

$$N_{OL} = (6.29 + 31.7P^2 + 0.23\ N_{np})^{0.5} \quad \text{(Eq. 3)}$$

American operators are paid 438% more than the operators at this facility which allowed us to use known sources of operator pay in order to estimate the operating cost of labor [1]. Table 12 depicts the results of the equation above along with the operator pay estimate. The 16 operators necessary is an overestimate since some operators can overlap on plant responsibilities, but this allows for a conservative economic estimate and a high degree of safety if no established operators are available to overlap. This also allows a cushion if any individuals miss work unexpectedly or due to lost time. In a more established and experienced facility, these costs will go down. Operator costs are constant for streams K and TQ1.

Table 12: Labor Costs

Required Operators	
Vessels	5
Pumps	4
Reactors	3
Fired Heater	1
Heat Exchangers	13
Towers	7
Compressors	1
Total Equipment	34
Equipment that Needs an Operator	25
N_{oL}	3.47
Total Number of Operators Required	16
Operator Pay per hour ($)	7.52
Operator Cost ($/yr)	$217,000

Utility costs have the second greatest impact on the operating costs behind raw materials. The process operating conditions allow the operators to use all utilities currently on site. Available utilities with their given cost are below in Table 13. Utility costs for each piece of equipment for stream K are listed below in Tables 14-18. Utility costs for each piece of equipment for stream TQ1 are listed below in Tables 19-23 The team determined these costs through common equations for utility costing [1] [4].

Table 13: Available Utility Costs

Utility	Cost
Electricity	$ 0.25 kWh
Steam, 450 psig	$19.36/1000 kg
Steam, 150 psig	$14.08/1000 kg
Steam, 50 psig	$8.80/1000 kg
Natural Gas	$9.43/MMBtu
Cooling Water, 25°C	$0.5/GJ

Table 14: Cooling Water Costs (K)

Equipment	Cost
E-102	$1,140,000
E-103	$3,200
E-105	$23,400
E-106	$12,800
E-107	$9,860
E-109	$15,700
E-111	$22,600
E-113	$8,860
Total	$1,230,000

Table 17: 150 psig steam Costs (K)

Equipment	Cost
E-104	$268,000
E-110	$309,000
E-112	$105,000
E-114	$123,000
Total	$804,000

Table 20: Electricity Costs (TQ1)

Equipment	Cost
P - 101 A/B	$82,400
P - 102 A/B	$2,610
P - 103 A/B	$2,920
P - 104 A/B	$823
P - 105 A/B	$1,470
K - 101	$2,430,000
Total	$2,520,000

Table 15: Electricity Costs (K)

Equipment	Cost
P - 101 A/B	$59,000
P - 102 A/B	$6,280
P - 103 A/B	$6,020
P - 104 A/B	$1,990
P - 105 A/B	$3,750
K - 101	$2,900,000
Total	$2,980,000

Table 16: Natural Gas Costs (K)

Equipment	Cost
E-101	$21,200,000

Table 18: 450 psig Steam Costs (K)

Equipment	Cost
E-108	$785,000

Table 19: Cooling Water Costs (TQ1)

Equipment	Cost
E-102	$1,250,000
E-103	$4,930
E-105	$29,200
E-106	$18,500
E-107	$4,420
E-109	$15,900
E-111	$6,230
E-113	$2,940
Total	$1,330,000

Table 21: Natural Gas Costs (TQ1)

Equipment	Cost
E-101	$23,028,234

Table 23: 450 psig Steam Costs (TQ1)

Equipment	Cost
E-108	$897,167

Table 22: 150 psig steam Costs (TQ1)

Equipment	Cost
E-104	$317,096
E-110	$234,800
E-112	$84,619
E-114	$40,701
Total	$677,217

Costs are based on the necessary flow of utility to each piece of equipment. Energy required by the water stream is crucial for calculating the operating cost of condensers. This information is provided by the Aspen Hysys software. Specific heat of vaporization is used to calculate mass flow rate of steam into the reboilers once the duty was retrieved from Aspen Hysys. The operating cost associated with pumps is the result of purchased horsepower. Once the head of the pump (ft) and flow rate (lb/hr) are determined, the purchased horsepower is calculated and thus converted into kilowatts. Electricity is also necessary in our compressor, K-101, which receives its power from a drive. Calculation of the brake horsepower is necessary for this cost. Natural gas costs are determined through analysis of the duty of E-101 provided by the simulation software and then used the costing per unit of energy for the utility.

Once all these analyses are done our manufacturing costs are set. Further manufacturing costs are derived using multiplication factors once key manufacturing costs are defined. Results of this summation are shown below in Tables 24 and 25. These costs may escalate in future years, but sensitivity analysis will analyze such effects in a later section.

Table 24: Manufacturing Costs (K)

Manufacturing Element	Cost
Raw Materials	$287,000,000
Waste Treatment	$4,520,000
Utilities	$27,000,000
Operating Labor	$217,000
Direct Supervisory and Clerical Labor	$39,000
Maintenance and Repairs	$8,940,000
Operating Supplies	$1,340,000
Laboratory Charges	$32,500
Patents and Royalties	$12,600,000
Direct Manufacturing Costs	**$342,000,000**
Local Taxes and Insurance	$4,770,000
Plant Overhead Costs	$5,520,000
Fixed Manufacturing Costs	**$10,300,000**
Administration Costs	$1,380,000
Distribution and Selling Costs	$46,300,000
Research and Development	$21,100,000
General Expenses	**$68,800,000**
Cost of Manufacture	**$421,000,000**

Table 25: Manufacturing Costs (TQ1)

Manufacturing Element	Cost
Raw Materials	$334,000,000
Waste Treatment	$4,650,000
Utilities	$28,300,000
Operating Labor	$217,000
Direct Supervisory and Clerical Labor	$39,000
Maintenance and Repairs	$8,940,000
Operating Supplies	$1,340,000
Laboratory Charges	$32,500
Patents and Royalties	$14,400,000
Direct Manufacturing Costs	**$391,000,000**
Local Taxes and Insurance	$4,770,000
Plant Overhead Costs	$5,520,000
Fixed Manufacturing Costs	**$10,300,000**
Administration Costs	$1,380,000
Distribution and Selling Costs	$52,800,000
Research and Development	$24,000,000
General Expenses	**$78,200,000**
Cost of Manufacture	**$480,000,000**

DCFROR Analysis

The project assumed a 15% minimum rate of return since one was not provided in the initial memorandum. Two tax rates were evaluated: a 35% tax rate under Iraqi control and a 15% tax rate under Kurdish control. Further assumptions include a five-year project evaluation life and a modified accelerated cost recovery system, MACRS, to determine depreciation costs. MACRS depreciation is a more robust model and factors in the benefits of straight line and double declining rate. The MACRS depreciation life is 10 years for oil refining equipment [2]. All remaining depreciation value was written off at the end of the project evaluation life.
The discounted cash flow rate of return, DCFROR, and the net present value, NPV, can determine a project's attractiveness. Attractive projects have a DCFROR greater than the minimum rate of return and an NPV greater than zero. Tables 26-27 show cash flow tables for stream K, while tables 28-29 depict cash flow for stream TQ1. The team assumed half-year production for year 2022 with full year production occurring in years 2023-2026. The project

writes off working capital at the end of evaluation life and includes reactor catalysts within working capital. Table 30 communicates depreciation factors for each year.

The refinery update employs a washout assumption to keep a constant revenue to expense margin. It also assumes escalation of costs and revenues to increase at different rates but by the same numerical value to keep a constant difference between the two values. Our team analyzed the economics based off a 5-year project evaluation life. The project memorandum provided no evaluation life; therefore, our team wanted to be conservative in our estimates to ensure a profitable process.

Table 26:	Cash Flow Table (Feed K: Iraqi Control)					
Corporate financial situation:	Expense					
Minimum rate of return, i*=	0.15	or	15	%		
Other Relevant Project Info:	Project Life 5 Year	MACRS	**Assume Washout**			
1=$1						
End of Year	2021	2022	2023	2024	2025	2026
Production "units"		402,000,000	805,000,000	805,000,000	805,000,000	805,000,000
x Sales Price, $/unit						
Sales Revenue		402,000,000	805,000,000	805,000,000	805,000,000	805,000,000
+Salvage Value						
-Royalties						
Net Revenue		402,000,000	805,000,000	805,000,000	805,000,000	805,000,000
-Raw Material Costs		-144,000,000	-287,000,000	-287,000,000	-287,000,000	-287,000,000
-Other Op Costs		-67,000,000	-134,000,000	-134,000,000	-134,000,000	-134,000,000
-Depreciation		-15,100,000	-27,100,000	-21,700,000	-17,400,000	-13,900,000
-Amortization						
-Depletion						
-Loss Forward						
-Writeoff						-77,400,000
Taxable Income		177,000,000	356,000,000	362,000,000	366,000,000	292,000,000
-tax @ 35%		-61,800,000	-125,000,000	-127,000,000	-128,000,000	-102,000,000
Net Income		115,000,000	232,000,000	235,000,000	238,000,000	190,000,000
+Depreciation		15,100,000	27,100,000	21,700,000	17,400,000	13,900,000
+Amortization						
+Depletion						
+Loss Forward						
+Writeoff						77,400,000
-Working Capital		-21,900,000				
-Fixed Capital	-151,000,000					
Cash Flow	-151,000,000	108,000,000	259,000,000	257,000,000	255,000,000	281,000,000
Discount Factor (P/F)	1.00	0.8696	0.7561	0.6575	0.5718	0.4972
Discounted Cash Flow	-151,000,000	93,900,000	196,000,000	169,000,000	146,000,000	140,000,000
NPV @ i* (15%)	594,000,000					
DCFROR	115%					
Payback Period (Years)	1.16					
DC Payback Period (Years)	1.29					

Table 27:	Cash Flow Table (Feed K: Kurdish Control)					
Corporate financial situation:	Expense					
Minimum rate of return, i*=	0.15	or	15	%		
Other Relevant Project Info:	Project Life 5 Year	MACRS	**Assume Washout**			
1=$1						
End of Year	2021	2022	2023	2024	2025	2026
Production "units"		402,000,000	805,000,000	805,000,000	805,000,000	805,000,000
x Sales Price, $/unit						
Sales Revenue		402,000,000	805,000,000	805,000,000	805,000,000	805,000,000
+Salvage Value						
-Royalties						
Net Revenue		402,000,000	805,000,000	805,000,000	805,000,000	805,000,000
-Raw Material Costs		-144,000,000	-287,000,000	-287,000,000	-287,000,000	-287,000,000
-Other Op Costs		-67,000,000	-134,000,000	-134,000,000	-134,000,000	-134,000,000
-Depreciation		-15,100,000	-27,100,000	-21,700,000	-17,400,000	-13,900,000
-Amortization						
-Depletion						
-Loss Forward						
-Writeoff						-77,400,000
Taxable Income		177,000,000	356,000,000	362,000,000	366,000,000	292,000,000
-tax @ 15%		-26,500,000	-53,500,000	-54,300,000	-54,900,000	-43,800,000
Net Income		150,000,000	303,000,000	307,000,000	311,000,000	248,000,000
+Depreciation		15,100,000	27,100,000	21,700,000	17,400,000	13,900,000
+Amortization						
+Depletion						
+Loss Forward						
+Writeoff						77,400,000
-Working Capital		-21,900,000				
-Fixed Capital	-151,000,000					
Cash Flow	-151,000,000	143,000,000	330,000,000	329,000,000	329,000,000	340,000,000
Discount Factor (P/F)	1.00	0.8696	0.7561	0.6575	0.5718	0.4972
Discounted Cash Flow	-151,000,000	125,000,000	250,000,000	216,000,000	188,000,000	169,000,000
NPV @ i* (15%)	797,000,000					
DCFROR	143%					
Payback Period (Years)	1.02					
DC Payback Period (Years)	1.10					

Table 28:	Cash Flow Table (Feed TQ1: Iraqi Control)					
Corporate financial situation:	Expense					
Minimum rate of return, i^*=	0.15	or	15	%		
Other Relevant Project Info:	Project Life 5 Year	MACRS	**Assume Washout**			
1=$1						
End of Year	2021	2022	2023	2024	2025	2026
Production "units"		607,000,000	1,210,000,000	1,210,000,000	1,210,000,000	1,210,000,000
x Sales Price, $/unit						
Sales Revenue		607,000,000	1,210,000,000	1,210,000,000	1,210,000,000	1,210,000,000
+Salvage Value						
-Royalties						
Net Revenue		607,000,000	1,210,000,000	1,210,000,000	1,210,000,000	1,210,000,000
-Raw Material Costs		-167,000,000	-334,000,000	-334,000,000	-334,000,000	-334,000,000
-Other Op Costs		-73,400,000	-147,000,000	-147,000,000	-147,000,000	-147,000,000
-Depreciation		-15,100,000	-27,100,000	-21,700,000	-17,400,000	-13,900,000
-Amortization						
-Depletion						
-Loss Forward						
-Writeoff						-77,400,000
Taxable Income		351,000,000	706,000,000	711,000,000	715,000,000	641,000,000
-tax @ 35%		-123,000,000	-247,000,000	-249,000,000	-250,000,000	-224,000,000
Net Income		228,000,000	459,000,000	462,000,000	465,000,000	417,000,000
+Depreciation		15,100,000	27,100,000	21,700,000	17,400,000	13,900,000
+Amortization						
+Depletion						
+Loss Forward						
+Writeoff						77,400,000
-Working Capital		-21,900,000				
-Fixed Capital	-151,000,000					
Cash Flow	-151,000,000	222,000,000	486,000,000	484,000,000	482,000,000	508,000,000
Discount Factor (P/F)	1.00	0.8696	0.7561	0.6575	0.5718	0.4972
Discounted Cash Flow	-151,000,000	193,000,000	367,000,000	318,000,000	276,000,000	253,000,000
NPV @ i* (15%)	1,260,000,000					
DCFROR	204%					
Payback Period (Years)	0.85					
DC Payback Period (Years)	0.89					

Table 29:	Cash Flow Table (Feed TQ1: Kurdish Control)					
Corporate financial situation:	Expense					
Minimum rate of return, i*=	0.15	or	15	%		
Other Relevant Project Info:	Project Life 5 Year	MACRS	**Assume Washout**			
1=$1						
End of Year	2021	2022	2023	2024	2025	2026
Production "units"		607,000,000	1,210,000,000	1,210,000,000	1,210,000,000	1,210,000,000
x Sales Price, $/unit						
Sales Revenue		607,000,000	1,210,000,000	1,210,000,000	1,210,000,000	1,210,000,000
+Salvage Value						
-Royalties						
Net Revenue		607,000,000	1,210,000,000	1,210,000,000	1,210,000,000	1,210,000,000
-Raw Material Costs		-167,000,000	-334,000,000	-334,000,000	-334,000,000	-334,000,000
-Other Op Costs		-73,400,000	-147,000,000	-147,000,000	-147,000,000	-147,000,000
-Depreciation		-15,100,000	-27,100,000	-21,700,000	-17,400,000	-13,900,000
-Amortization						
-Depletion						
-Loss Forward						
-Writeoff						-77,400,000
Taxable Income		351,000,000	706,000,000	711,000,000	715,000,000	641,000,000
-tax @ 15%		-52,700,000	-106,000,000	-107,000,000	-107,000,000	-96,200,000
Net Income		299,000,000	600,000,000	604,000,000	608,000,000	545,000,000
+Depreciation		15,100,000	27,100,000	21,700,000	17,400,000	13,900,000
+Amortization						
+Depletion						
+Loss Forward						
+Writeoff						77,400,000
-Working Capital		-21,900,000				
-Fixed Capital	-151,000,000					
Cash Flow	-151,000,000	292,000,000	627,000,000	626,000,000	625,000,000	637,000,000
Discount Factor (P/F)	1.00	0.8696	0.7561	0.6575	0.5718	0.4972
Discounted Cash Flow	-151,000,000	254,000,000	474,000,000	412,000,000	358,000,000	316,000,000
NPV @ i* (15%)	1,660,000,000					
DCFROR	256%					
Payback Period (Years)	0.77					
DC Payback Period (Years)	0.78					

Table 30: MACRS Depreciation

MACRS 10 Year Property	
Year 1	0.1
Year 2	0.18
Year 3	0.144
Year 4	0.1152
Year 5	0.0922
Year 6	0.0737
Year 7	0.0655
Year 8	0.0655
Year 9	0.0656
Year 10	0.0655
Year 11	0.0328

The cash flow sheets depict the highest NPV at $1,660,000,000 to be with stream TQ1 and Kurdish taxes. The lowest NPV is $594,000,000 seen at stream K and Iraqi taxes. Therefore, all four cash flow sheets are economically favorable. No pay back periods exceed 2 years. Since cash flow is positive this project is revenue producing. The discrepancy in taxes and revenue streams account for the difference between the 4 cash flow sheets. The project optimized Aspen Hysys to limit operating costs and maximize the most lucrative product streams. This was all in an effort to maximize the NPV and DCFROR.

In order for each of these streams to be economically attractive with their respective tax rates, they must have an NPV greater than 0. The breakeven revenue necessary for each year of the project evaluation life is listed below in Table 31.

Table 31: Breakeven Revenue

Initial Capital Investment	Breakeven Revenue
$151,000,000	$44,500,000

Sensitivity Analysis

Numerous variables affect the NPV for the process. While all estimates made are conservative, variance in costs could occur if this process moves forward. In order to estimate how these variances could affect the economic attractiveness of the project, the overhaul varies multiple costs positively and negatively. The degree to which each cost is varied is based on expected variances in industry from published literature [1]. Annual profit, initial capital investment, raw material cost, and operating costs are all varied in an effort to examine as many factors that could affect the NPV as reasonable. Single variable sensitivity analysis is done for each of these factors. Each factor varies between its lowest expected and highest expected value keeping all other variables constant. This method accounts for project uncertainty but fails to take into account probability [1]. Tornado charts depicted below in Figures 4-7 show the results of this analysis for each stream and tax regime combination. Annual profit shows the greatest variation in NPV, but is also varied the most. Raw material costs are expected to affect the process economics the most [1]. Based on our figures, raw material costs affect the process the second-most following annual profit. The initial capital investment affect the NPV value the least in each figure. The utilities show such little variation by comparison since the raw material costs and revenue are much larger in value.

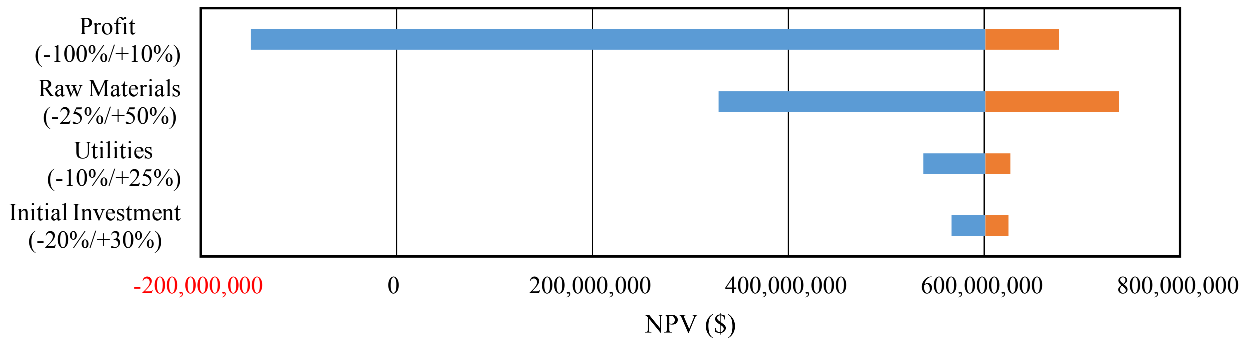


Figure 4: Tornado Chart for Stream K: Iraqi Taxes

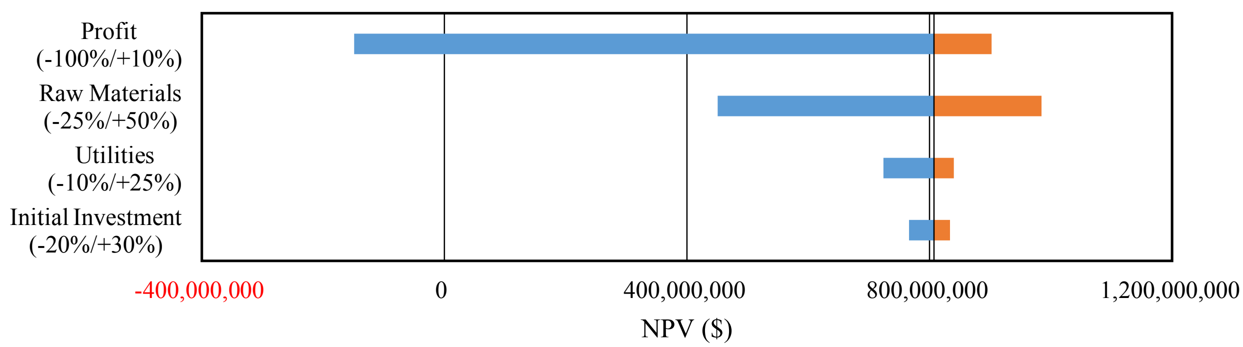


Figure 5: Tornado Chart for Stream K: Kurdish Taxes

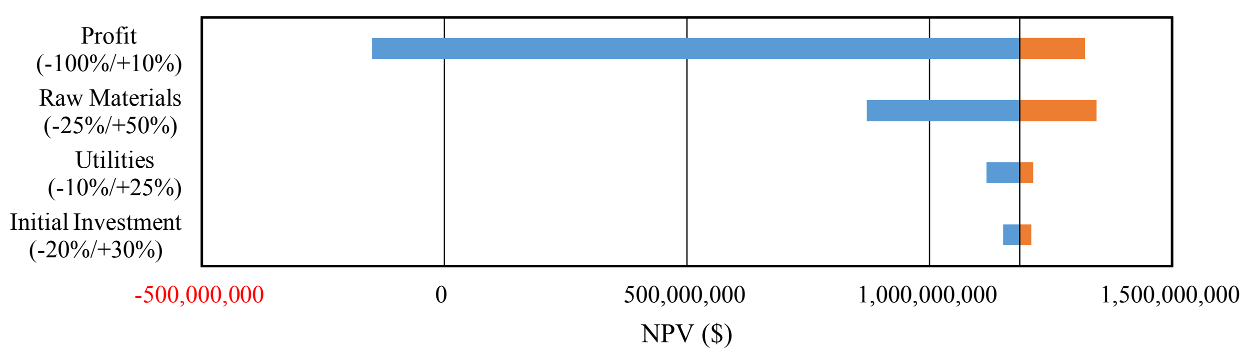


Figure 6: Tornado Chart for Stream TQ1: Iraqi Taxes

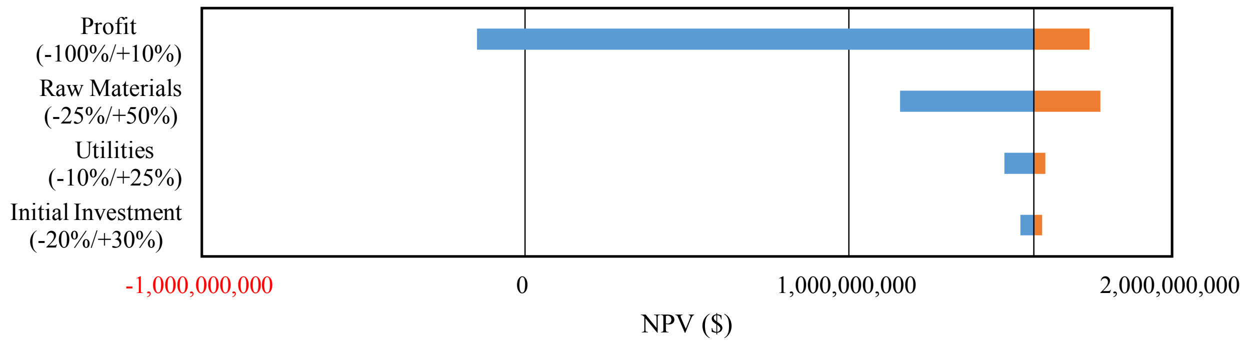


Figure 7: Tornado Chart for Stream TQ1: Kurdish Taxes

In the tornado charts above, each variable is isolated and varied. Below in Table 32 each variable is manipulated to produce the best and worst NPV possible together. Best case scenario minimized all costs and maximized profit. Worst case scenario is understandably the opposite approach. Project evaluation life is kept constant at 5 years.

Table 32: Best- and Worst-Case Scenarios

Feed	Tax Rate	Worst Case Scenario	Expected Case	Best Case Scenario
K	35%	-$194,000,000	$594,000,000	$877,000,000
	15%	-$194,000,000	$797,000,000	$1,160,000,000
TQ1	35%	-$194,000,000	$1,260,000,000	$1,550,000,000
	15%	-$194,000,000	$1,660,000,000	$2,040,000,000

In order to measure quantitative risk, Monte Carlo methods are utilized. Monte Carlo varied potential scenarios ranging from best to worst case scenario. NPVs are calculated for 501 random samples for each potential stream and tax rate. The principle of the *Central Limit Theory* influenced the method used. *Central Limit Theory* states that unlimited samples will be normally distributed [1]. Since our sample size is so large, normal distribution is assumed. Figure 8 shows results from the Monte Carlo for feed K and Iraqi taxes at 35%. The normal distribution is seen in the central tendency of the bars.

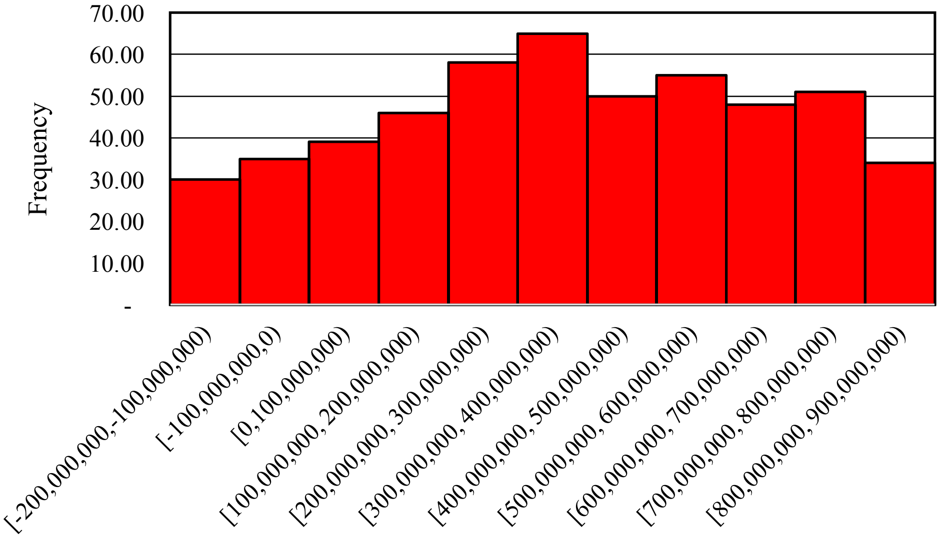


Figure 8: Monte Carlo for Feed K: Iraqi Taxes

Results from all 4 Monte Carlo analyses are seen below in Table 33. Projects that were economically favorable have an NPV greater than 0. Feed TQ1 under Kurdish taxes produces the highest proportion of favorable projects, while feed K produces the lowest proportion under Iraqi taxes.

Table 33: Monte Carlo Results

Stream	Tax Rate	% of NPV > 0	Average NPV
K	35%	79.6%	$336,000,000
	15%	84.8%	$466,000,000
TQ1	35%	86.8%	$502,000,000
	15%	91.4%	$909,000,000

Environment, Health, and Safety

Introduction

The aspects of environment, health, and safety are critically important to the economic viability, sustainability, and social responsibility of chemical sector investment and operations. For preliminary design, the relative cost and effort required to analyze hazards and take the preventative steps necessary in the design of the plant is minimal compared to the construction and operation of the plant. It is pertinent that the plant is designed and operated within the requirements of the Occupational Safety & Health Administration Process Safety Management (OSHA PSM), which is inside the fence line of the plant, and also the Environmental Protection Agency Risk Management Plan (EPA RMP), which is outside of the plant fence line. This section highlights the inherently safer design factors and the process safety management factors considered in preliminary design to ensure compliance and risk minimization for Mr. Abbasi's toppings refinery.

Inherent Safety Evaluation

The approach of inherently safer design aims to recognize and prevent risk by establishing foundationally safer characteristics throughout the plant. The ways in which equipment can be made inherently safer lie in four methods: substitution, minimization, moderation, and simplification. While simplification focuses on substituting a hazardous material with a less hazardous alternative, minimization aims to limit quantities of hazardous substances by storage; moderation looks at operating under less hazardous conditions by lowering pressure and temperature, and simplification involves minimizing unnecessary complexity in the plant by reducing equipment or by other methods.

In the area of substitution, the design group recognized one main area of the plant design that could be managed moving forward to further achieve an inherently safer design regarding both process safety and environmental safety. According to the chart of chemical exposure limits, Table 36, chemicals in this process are most hazardous when in contact with oxygen. Replacing natural gas in the fired heater would minimize this exposure to oxygen, and therefore, provide an inherently safer fired heater in the reactions section of the plant. According to recent study, hydrogen has been used as a substitute to natural gas in the design of a burner for fired heaters [5]. By utilizing this method, the fired heater would be allowed to operate by using less hazardous material and would reduce the carbon footprint of the plant.

An area to focus on minimization in the plant lies in the storage of sulfolane material. Since the sulfolane stream incorporates several hazardous materials, storage of this material must be managed and minimized to contribute to an overall inherently safer design. Therefore, the shipments of sulfolane material could be set to arrive twice a week. This would allow for less quantities of sulfolane to be present at the plant at all times, thus minimizing the risk involved with large amounts of hazardous material storage. The storage of the platinum catalyst used in the plugged flow reactors will also be minimized. In case of an urgent need of fresh catalyst, only enough catalyst will be stored onsite to refill the largest reactor. Otherwise, the catalyst will be ordered upon request. Table 34 provides the storage amounts of all materials within the refinery.

Table 34: Chemical Inventory

Chemical	Symbol	Amount (lb)	Amount (lb/day)
Sulfolane	$C_4H_8SO_2$	760,000	216,000
Platinum Catalyst	-	38,000	-
Air	-	Not Stored	254,000
Water	H_2O	Not Stored	43,200

As part of the plant's moderation, several considerations have been made concerning pressure profiles, particularly regarding the major fractionator. As the plant was originally designed to use a high tray pressure, the overhaul reduces the pressure drop to 0.1 psi per tray. This allowed for more accurate separation within the columns. The lowering of tray pressure also eliminated large pressure drops between trays, which is a large contributor to the overall inherent safety of the process. Moreover, the redesign keeps the pressures of the vessels and towers apart from the major fractionator to a minimum to ensure separation could be made under less hazardous conditions.

To simplify the process, the design group focused on the extraction section of the plant, which involves the largest amount of equipment. While simulating the plant based on the block flow diagram given in the project memorandum, the team determined that the absorption column following the second extractor was not providing enough separation of water from the sulfolane recycle stream. Therefore, the group's design removed this vessel to eliminate unnecessary complexity. In this way, the products of the second extractor are a product stream, consisting of large hydrocarbons sent to sales, and a waste stream. This subtraction also removed a reboiler process. In order to remove all of the water from the sulfolane recycle stream, the duty on this reboiler would have been exponentially high causing high risk heat transfer to take place. The takeout of this column allows for the plant to achieve the same desired results while using less pieces of equipment, helping us achieve an overall inherently safer design.

Process Safety Management Considerations

When designing a chemical refining process, designers must know the properties of the chemicals being used as well as how they react with each other when they are combined, whether that be by design or not. Considering temperature and pressure operating conditions, other than the use of the fired heater, the process operates within the operating envelope of 0-150 psig and 100-500 °F. The process stream reaches around 950 °F in the fired heater. The temperature must be this high so there is an effective conversion within the reactors. Since this is outside of the operating envelope, the hazards accompanying high temperatures should be considered, such as a higher risk of fires and loss of containment. The most important factor to consider is the safety of the public and environment.

Process Hazards

The physical properties of chemicals are very important in understanding how they will act in certain scenarios. Table 35 contains properties of the chemicals used in this process. Knowing the properties of these chemicals is helpful in determining the consequences in a loss of containment scenario as well as the procedures required for a specific situation.

Table 35: Materials Properties

	Benzene	Butane	Carbon Dioxide	Carbon Monoxide	Cyclohexane
Flash Point (°F)	12.0	-76.0	Data Unavailable	Data Unavailable	-4.0
Lower Explosive Limit	1.4%	1.9%	Data Unavailable	12.0%	1.3%
Upper Explosive Limit	8.0%	8.5%	Data Unavailable	75.0%	8.4%
Autoignition Temperature (°F)	1097.0	550.0	Data Unavailable	1128.0	518.0
Vapor Pressure (mmHg)	76 @ 68°F	760 @31.1°F	42940.0	> 26600	95 @ 68°F
Vapor Density (Relative to Air)	2.8	2.0	Data Unavailable	Data Unavailable	2.9
Specific Gravity (32°F)	0.879 @ 68°F	0.6 @32°F	1.56 @ -110.2°F	0.791 @-312.7°F	0.779 @ 68°F
Boiling point (760 mmHg)	176.2	31.1	Sublimes	-312.7	177.3
Molecular weight	78.1	58.1	44.0	28.0	84.2
Reactivity With Air	Highly Flammable	Highly Flammable	N/A	Highly Flammable	Highly Flammable
Reactivity With Water	Slightly Soluble	Insoluble	Soluble	Soluble	Insoluble
OSHA PEL	10 ppm	800 ppm	5000 ppm	35 ppm	300 ppm
LD_{50}	6.5 mL/kg/4h	65800 mg/m3	N/A	3760 ppm	70000 mg/m3/2h

	Ethane	Hydrogen	Methane	N-Decane	N-Heptane
Flash Point (°F)	-211.0	Data Unavailable	-306.0	115.0	25.0
Lower Explosive Limit	2.9%	4.0%	5.0%	0.8%	1.0%
Upper Explosive Limit	13.0%	75.0%	15.0%	2.6%	7.0%
Autoignition Temperature (°F)	940.0	1065.0	1004.0	410.0	433.0
Vapor Pressure (mmHg)	Data Unavailable	Data Unavailable	258574 @ 100°F	2.7 @ 68°F	37.49 @ 70°F
Vapor Density (Relative to Air)	1.0	Data Unavailable	0.6	4.9	3.5
Specific Gravity (32°F)	0.546 @ -127.5°F	0.071 @ -432.4°F	0.422 @ -256°F	0.73 @ 60°F	0.6838 @ 68°F
Boiling point (760 mmHg)	-127.5	-423.0	-258.7	345.4	209.1
Molecular weight	30.1	2.0	16.0	142.3	100.2
Reactivity With Air	Highly Flammable	Highly Flammable	Highly Flammable	Highly Flammable	Highly Flammable
Reactivity With Water	Insoluble	N/A	Insoluble	Insoluble	Insoluble
OSHA PEL	N/A	N/A	N/A	500 ppm	400 ppm
LD_{50}	N/A	N/A	N/A	72.3 mg/L/4h	103 g/m3/4h

	N-Hexane	N-Nonane	N-Octane	N-Pentane	Nitrogen
Flash Point (°F)	-9.4	88.0	56.0	-57.0	Data Unavailable
Lower Explosive Limit	1.2%	0.8%	1.0%	1.5%	Data Unavailable
Upper Explosive Limit	7.5%	2.9%	6.5%	7.8%	Data Unavailable
Autoignition Temperature (°F)	437.0	401.0	428.0	500.0	Data Unavailable
Vapor Pressure (mmHg)	120 @ 68°F	3.22 @ 68°F	10.0	400 @ 65.3°F	Data Unavailable
Vapor Density (Relative to Air)	3.0	4.4	3.9	2.5	Data Unavailable
Specific Gravity (32°F)	0.659 @ 68°F	0.718 @ 68°F	0.703 @ 68°F	0.626 @ 68°F	0.807 @ -319.9°F
Boiling point (760 mmHg)	156.0	303.4	258.1	97.0	-320.1
Molecular weight	86.2	128.3	114.2	72.2	28.0
Reactivity With Air	Highly Flammable	Highly Flammable	Highly Flammable	Highly Flammable	N/A
Reactivity With Water	Insoluble	Insoluble	Insoluble	Insoluble	Slightly Soluble
OSHA PEL	500 ppm	200 ppm	500 ppm	1000 ppm	N/A
LD_{50}	150 g/m3/2h	3200 ppm/4h	118 g/m3/4h	364 g/m3/4h	N/A

	Oxygen	P-Xylene	Propane	Sulfolane	Toluene
Flash Point (°F)	Data Unavailable	81.0	-156.0	330.0	40.0
Lower Explosive Limit	Data Unavailable	1.1%	2.1%	Data Unavailable	1.3%
Upper Explosive Limit	Data Unavailable	7.0%	9.5%	Data Unavailable	7.1%
Autoignition Temperature (°F)	Data Unavailable	984.0	842.0	Data Unavailable	896.0
Vapor Pressure (mmHg)	Data Unavailable	10 @ 81.1°F	9823.0	Data Unavailable	20 @ 65.1°F
Vapor Density (Relative to Air)	Data Unavailable	3.7	1.5	Data Unavailable	3.1
Specific Gravity (32°F)	1.14 @ -297.4°F	0.861 @ 68°F	0.59 @ -58°F	1.26 @ 86°F	0.867 @ 68°F
Boiling point (760 mmHg)	-297.3	280.9	-43.8	545.0	231.1
Molecular weight	32.0	106.2	44.1	120.2	92.1
Reactivity With Air	N/A	Highly Flammable	Highly Flammable	N/A	Highly Flammable
Reactivity With Water	N/A	Insoluble	Insoluble	Soluble	Insoluble
OSHA PEL	N/A	50 ppm	1000 ppm	0.37 ppm	200 ppm
LD_{50}	N/A	19.8 mg/L/4h	N/A	12 g/m3/4h	49 g/m3/4h

As discussed previously, it is very important to understand how chemicals will react when combined, whether that be by design or by mistake. The Chemical Reactivity Worksheet software [6] was used to compile a chemical compatibility matrix of all the chemicals used within the process and can be found in Table 36. This table also highlights the NFPA flammability, instability, health, and safety classifications of each chemical. For this process, the only incompatibility is any hydrocarbon with the presence of oxygen. The oxygenation of hydrocarbons leads to a large flammability risk. All that is needed is an ignition source when oxygen and hydrocarbons are mixed. The fired heater is the only unit that requires air flow, so the potential of a hydrocarbon and oxygen mixture is limited since the process is kept within the pipes.

Table 36: Chemical Compatibility Matrix

Health	Flammability	Instability	Special	Chemical Reactivity Compatibility Chart	Benzene	Butane	Carbon Dioxide	Carbon Monoxide	Cyclohexane	Ethane	Hydrogen	Methane	N-Decane	N-Heptane	N-Hexane	N-Nonane	N-Octane	N-Pentane	Nitrogen	Oxygen	P-Xylene	Propane	Sulfolane	Toluene	Water
2	3	0		Benzene																					
1	4	0		Butane	Y																				
				Carbon Dioxide	Y	Y																			
3	4	0		Carbon Monoxide	Y	Y	Y																		
1	3	0		Cyclohexane	Y	Y	Y	Y																	
1	4	0		Ethane	Y	Y	Y	Y	Y																
0	4	0		Hydrogen	Y	Y	Y	Y	Y	Y															
2	4	0		Methane	Y	Y	Y	Y	Y	Y	Y														
1	2	0		N-Decane	Y	Y	Y	Y	Y	Y	Y	Y													
1	3	0		N-Heptane	Y	Y	Y	Y	Y	Y	Y	Y	Y												
	3	0		N-Hexane	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y											
1	3	0		N-Nonane	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y										
1	3	0		N-Octane	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y									
1	4	0		N-Pentane	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y								
				Nitrogen	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y							
3	0	0	Oxidize	Oxygen	N	N	Y	N	N	N	N	N	N	N	N	N	N	N	Y						
2	3	0		P-Xylene	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N					
2	4	0		Propane	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y				
1	1	0		Sulfolane	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y			
2	3	0		Toluene	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y		
				Water	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	Y	N	Y	Y	Y	Y	

Chart Legend		
Y	:	Compatible
No hazardous reactivity issues expected		
N	:	Incompatible
Hazardous reactivity issues are expected		
C	:	Caution
May be hazardous under certain conditions		
SR	:	Self-Reactive
Potentially self-reactive (e.g., polymerizable)		

P&ID of the Major Fractionator

To ensure proper control of the Major Fractionator, our team developed a Process and Instrumentation Diagram for column T-103 which Figure 9 posits. This column yields the Reformate stream, which is composed of material for the final desired products. In the diagram, the design group positioned automatic control loops on several parts of the apparatus to monitor and control liquid level, pressure, and temperature. To minimize gaseous and liquid wastes, our team attached temperature controllers and indicators on several streams as well as on multiple stages of the distillation column. Furthermore, the design utilizes level controllers on the tower and the reflux drum to eliminate flooding. Pressure controllers on the top of the tower and on the distillate stream aim to keep the pressures at an acceptable level. The pressure controllers will also work to minimize risks of pressure buildups and explosions. The controller TI-107 leads to a monitored temperature and composition of the most important stream in the plant.

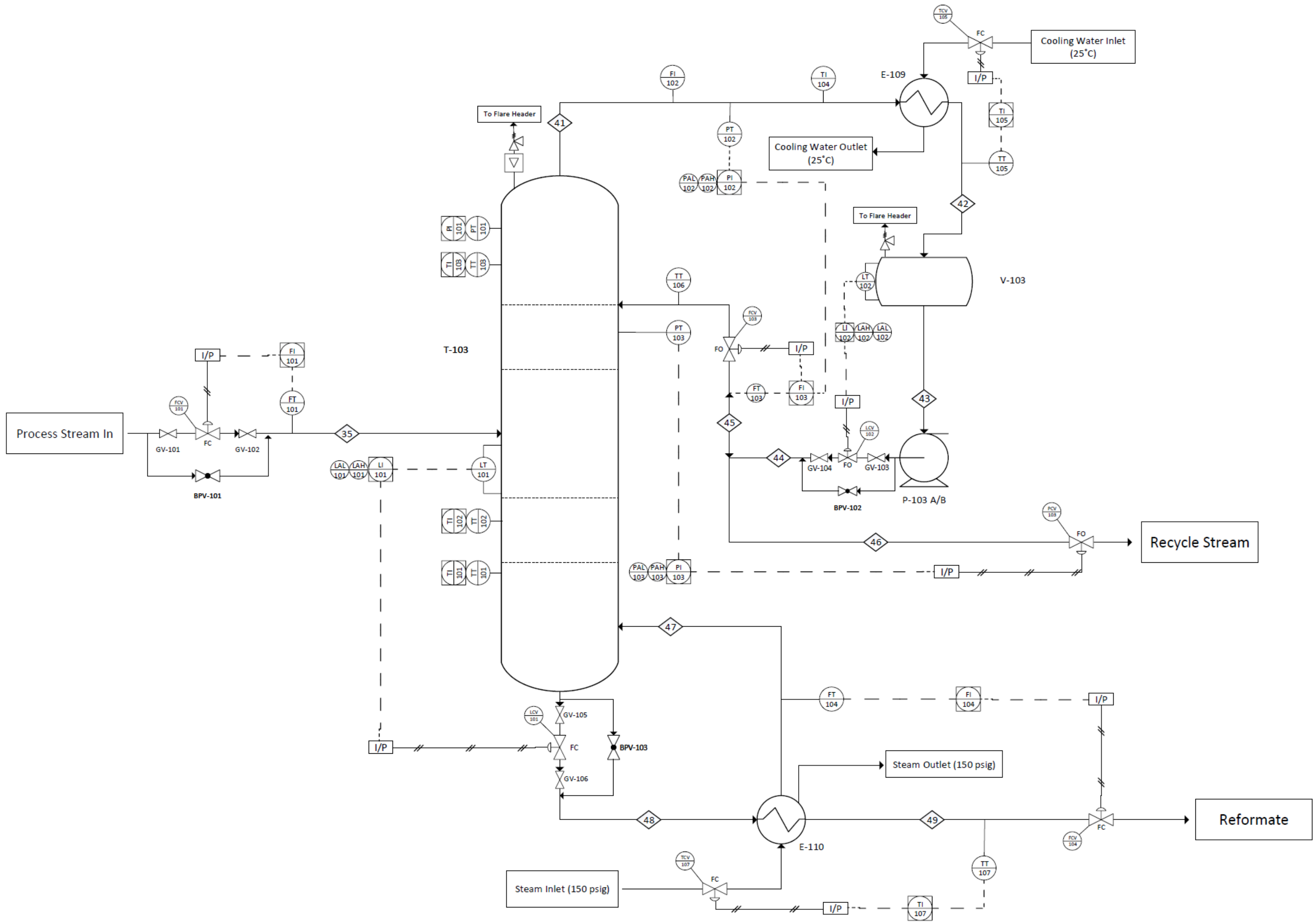


Figure 9: Major Fractionator P&ID

Pressure relief devices are present throughout the column to provide additional process safety such as a rupture disk and relief valve placed at the top of the tower, T-103, as a defense against high pressure. The reflux drum, V-103, also has a pressure relief valve. The project team sized pressure relief according to the American Petroleum Institute (API) standard *520 Sizing for Gas or Vapor Relief*, and the results are shown in Table 37. The discharge lines from all pressure relief valves lead to a flare header [7]. In order to maintain the integrity of the process equipment, it is recommended that the rupture disk installed on the tower be either in the zero or negative manufacturing range, so that there is a guarantee the disk will rupture at or slightly before the set pressure.

Table 37: PSV & Rupture Disk Sizing

	T-103 PSV	T-103 Rupture Disk	V-103 PSV
P_{set} (psia)	106.7	106.7	99
w (lb/hr)	11700	11700	21400
A (in^2)	1.20	1.89	2.34
Relief Valve designation	J	-	L
Inlet Diameter (in)	3	3	4
Outlet Diameter (in)	4	3	6

Uncongested Vapor Cloud Deflagration

The three most common chemical plant accidents are fires, explosions, and toxic releases. In order to prevent these accidents from occurring, engineers must be familiar with the fire and explosion properties of materials, the nature of the fire and explosion process, and procedures to reduce fire and explosion hazards. For the preliminary design of the toppings refinery, the plan calls for a TNT equivalency calculation to be performed for the atmospheric detonation of all chemicals from the largest process distillation column. Table 38 portrays this evaluation, where the total mass of TNT, using equation 4, is given as well as the scaled distance, Z_e, and scaled overpressure, p_0/p_a. Using Equation 5 and 6, respectively, the design team calculated the scaled distance and overpressure.

Overall, the side-on overpressure gives a summary of the damage which will occur at a specified distance away from the detonation of a specific mass of TNT. The blast map, which is shown in Figure 10, helps the team understand what damage to expect if an explosion were to occur. This figure also helps understand how far away to place feedstock and product storage, so one explosion doesn't start a chain link of explosions which could have been avoidable.

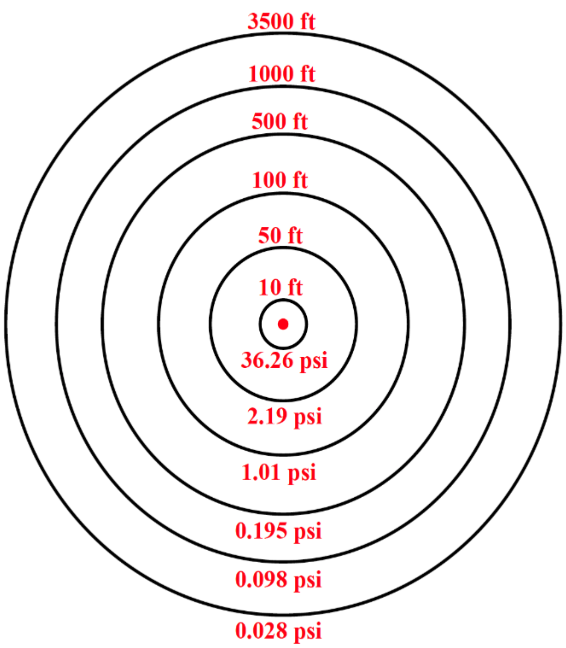
$$m_{TNT} = \frac{\eta m \Delta H_c}{E_{TNT}} \quad \text{(Eq. 4)}$$

$$z_e = \frac{r}{m_{TNT}^{1/3}} \quad \text{(Eq. 5)}$$

$$\frac{p_0}{p_a} = \frac{1616\,[1 + \left(\frac{z_e}{4.5}\right)^2]}{\sqrt{1 + (\frac{z_e}{0.048})^2}\sqrt{1 + (\frac{z_e}{0.32})^2}\sqrt{1 + (\frac{z_e}{1.35})^2}} \quad \text{(Eq. 6)}$$

Table 38: TNT equivalency

m_{TNT} (lb)	r (ft)	Z_e	p_0/p_a	scaled overpressure
4.03	10	2.492	2.467	36.255
	50	12.460	0.149	2.193
	100	24.920	0.068	1.006
	150	37.380	0.045	0.660
	200	49.841	0.033	0.492
	250	62.301	0.027	0.392
	300	74.761	0.022	0.326
	350	87.221	0.019	0.280
	400	99.681	0.017	0.244
	450	112.141	0.015	0.217
	500	124.602	0.013	0.195
	1000	249.203	0.007	0.098
	1500	373.805	0.004	0.065
	2000	498.406	0.003	0.049
	3000	747.610	0.002	0.033
	3500	872.211	0.002	0.028



Pressure (psi)	Damage
0.03	Occasional breaking of large class windows already under strain
0.1	Breakage of small windows under strain
0.3	"Safe distance" projectile limit; some damage to house ceilings; 10% window glass broken
1-2	Corrugated asbestos shatters; corrugated steel or aluminum panels, fastenings fail, followed by buckling; wood panels, fastenings fail, panels blow in
2-3	Concrete or cinder blocks walls, not reinforced, shatter
>10	Probable total destruction of buildings; heavy machine tools (7000 lb) moved and badly damaged, very heavy machine tools (12,000 lb) survive

Figure 10: TNT Equivalency Blast Map [8]

It is crucial to identify and mitigate potential hazards and risks before refineries begin operations. The process hazard analysis system ensures the adherence to industry and company standards. A common evaluation tool when working through a process hazard analysis is a "what-if" analysis. This is a systematic process which helps evaluate what can go wrong, the consequences that occur due to the issue, and how to address the risk with recommended changes. Table 39 is a "what-if" analysis for the major fractionator and assesses some potential scenarios and recommendations should these issues occur.

Table 39: Major Fractionator "What-if" Analysis

What if?	Likelihood	Hazard/ hazardous event	Consequence	Recommended action
Reflux level too low (V-103)	Likely	Not enough liquid to pump back into T-103/ Starting pump when level is too low	Process upset	Low Level alarm in V-103
Incorrect feed rate	Likely	Too much or not enough feed into T-103	Process upset	Flowmeter control loop on stream 35
Reflux pump failure (P-103 A)	Likely	Pump shutdown/Failure	Process upset	Backup pump should be available
Column overpressure scenario (T-103)	Likely	Continued build up of pressure within process	Process upset	Installed pressure relief on T-103
Valve LCV-101 closed	Unlikely	Increased liquid level in T-103/ Eventual backflow into feed line/ Eventual liquid in distillate stream	Process upset	High level alarm in T-103/ By-pass around LCV-101
Valve LCV-102 closed	Unlikely	No flow to recycle stream or back into T-103/ Pump overpressure	Process upset/ Broken pump seal	High level alarm in V-103/ PSV installation on discharge of P-103 A/B
Loss of steam in reboiler (E-110)	Unlikely	Loss of temperature & pressure control in T-103	Process upset	Low temperature alarm for stream 49
Loss of cooling water in condenser (E-109)	Unlikely	Loss of temperature & pressure control in T-103/ overpressure scenario in T-103 or V-103	Process upset	High temperature alarm on stream 42 and pressure relief devices installed for T-103 and V-103
Reflux drum overpressure with faulty PSV (V-103)	Very Unlikely	Overpressure within V-103	Process upset/ Possible loss of containment	Regular pressure relief device inspection
Both main and backup reflux pump failure (P-103 A/B)	Very Unlikely	No liquid leaving V-103	Process upset	High level alarm in V-103
Flame because of flammable liquid fire	Extremely Unlikely	Catastrophic tower failure	Loss of containment	Installation of flame detection in T-103

The potential consequences due to loss of containment or process explosions allow the design team to focus on risks that should be mitigated for both the company and the community in which it operates. Table 40 is a potential consequence summary should a loss of containment or explosion occur.

Table 40: Potential Consequence Summary

Hazard	Equipment Damage	Environmental Compliance	Loss of Life	Disruption of Other Business Units	Legal/PR	Community Impact
Benzene LOC	Medium	Medium	High	Low	Medium	Low
Toluene LOC	Medium	Medium	High	Low	Medium	Low
Xylene LOC	Medium	Medium	High	Low	Medium	Low
Reformate Explosion	High	Medium	Medium	Medium	High	Low

Conclusions

In order to meet new processing and refining standards while processing naphtha, the team designed the process given above. This report designed and costed all process units necessary to achieve this end.

In an effort to create an inherently safer design, the team's process eliminated an extra column considered for separating sulfolane and water for the purpose of recycling the sulfolane back into LLE-101 was eliminated from our process. This left capital costs incurred in 2021 to be around $151 million. The project utilizes a 10-year MACRS depreciation to depreciate the equipment. It also assumes washout for escalation of all revenues and costs. Revenues vary among the two different feed streams and two different tax regimes. Upon our economic analysis, all projects are attractive with discounted cash flow rates of return ranging from 115-256 % (far exceeding the minimum hurdle rate of 15%) and net present values' in year 2021 ranging from $594 million to $1.66 billion. The greatest economic return is expected for feed TQ1 under a Kurdish tax regime with the lowest economic return being expected for feed K under Iraqi tax control.

The design proposed varies expected costs and revenues in order to analyze any risks or potential market fluctuations that may occur. The team varied capital costs, utility costs, raw materials, and expected profit from a best to worst case scenario for each variable. The project's conclusions indicate a lack of profit would have the greatest effect on the NPV for any feed or tax regime. However, variance for profit is greater than that of raw material cost which is expected to have the greatest effect on project economics. In order to analyze multiple factors under quantitative analysis, the team employed Monte Carlo methods for this project for each feed and tax code. The success of any given project was measured as having an NPV > 0. Success ranged from 79.6-91.4 % for the different combinations. Our group is confident that from these findings we can conclude this project will be profitable.

When developing this project, safety received the highest amount of consideration. The design group identified and accounted for inherent safety principles of the plant, including methods of substitution, minimization, moderation, and simplification. The takeout of the recycle absorber after the second extraction column was the most prominent of these considerations. Furthermore, considerations in the area of process safety management allowed for the quantification of hazards regarding material properties, chemical compatibility, explosion risks, and potential consequences. The Process and Instrumentation Diagram allowed for alarmed controls to be placed on multiple streams involved in the major fractionator. From these measures, we employed two pressure relief valves and one rupture disk to allow for appropriate safety equipment to be in place. Altogether, the steps taken to analyze process hazards and prepare for potential areas of risk have allowed the design team to create an inherently safer process that is capable of operating in a safe and efficient manner.

Appendix

Reactors

The assumptions used in modeling are:

- the reactors can be modeled as plug flow reactors;
- the plant is operating continuously;
- the reactor can be costed as a horizontal vessel with packing;
- the pressure drop across the reactors was 5 psi.

For use of a swing reactor, the team picked the largest reactor for the spare reactor size. This allows for the substitution of any of the three reactors which will allow for the process to run continuously and not have to shut the plant down in the event of necessary spare usage. When substitution occurs, the reactor will be isolated to regenerate the catalyst to ensure all surfaces are active on the catalyst. To check for catalyst deactivation, a test should be run at least once a month to make sure all or most of the catalyst is still active.

The kinetic equations shown in Table 2 are used to determine the rate of reaction for each chemical reaction throughout the three reactor which use the temperature (K) and pressure (MPa) of the reactants to determine the rate in kmol/(m^3-hr). The parameters used for the kinetic equations are in Table 41.

Table 41: Kinetic Parameters

Kinetic Parameters	**Value (Units)**
T	Temperature of the reactor (Kelvin)
$P_{C_6H_{12}}$	Pressure of the C_6H_{12} in the reactor (MPa)
$P_{C_6H_6}$	Pressure of the C_6H_6 in the reactor (MPa)
P_{H_2}	Pressure of the H_2 in the reactor (MPa)
$P_{C_{10}H_{22}}$	Pressure of the $C_{10}H_{22}$ in the reactor (MPa)

The design operating temperature is 930°F since cracking works better in the gaseous state at high temperatures. The design calls for a 100 psia operating pressure for the first reactor, 95 psia for the second, and 90 psia for the third due to pressure drop through each reactor. The project chose a higher pressure, since the cracking reaction was determined to work better at higher pressures. Only 5% of the hydrogen is purged with the rest of the gaseous stream leaving V-101 recycled back to the R-101 feed stream. Increasing the hydrogen present in the reactors allows for increased cracking reactions to occur.

The reactor section includes three reactors, a fired heater, a compressor, a distillation column with a condenser, two vapor-liquid separators, a pump, and two more heat exchangers. The bare module capital cost for all equipment present in this section is listed above in Table 5 but is also detailed here below in Table 42.

Table 42: Bare Module Capital Cost – Reactor Section

Equipment	Cost
R - 101	$162,000
R - 102	$223,000
R - 103	$259,000
Catalyst	$683,000
V -101	$10,700
V -102	$9,970
T - 101	$492,000
E - 101	$138,000,000
E - 102	$278,000
E - 103	$145,000
E - 104	$94,200
K - 101	$1,750,000
P - 101 A/B	$33,700

In order to maintain the processing conditions, many utilities are necessary throughout the process equipment in this section. Tables 14-18 provide operating costs for each piece of equipment, but Table 43 itemizes the operating costs specific to the reactor section.

Table 43: Reactor Section Operating Costs for Stream K

Equipment	Cost
E - 101	$21,200,000
E - 102	$1,140,000
E - 103	$3,200
E - 104	$268,000
K - 101	$2,900,000
P - 101 A/B	$59,000
Labor	$78,000

Extraction

The liquid-liquid extractors remove chained alkane carbons from the product stream. Sulfolane is the top feed for LLE-101 to extract hydrocarbon chains. Water is the top feed for LLE-102 to extract the sulfolane through the bottom outlet stream so the top stream can be mainly hydrocarbons. For costing purposes, we modeled extractors as trayed vessels. Since sulfolane can become increasingly corrosive when mixed with water, the design uses stainless steel as the material of construction for LLE-102 as opposed to carbon steel used everywhere else in the process. One innovation enacted by our group involves treating the mixed sulfolane and water stream as waste rather than separate through a distillation column in order to recycle the sulfolane back into the extraction system. In order to build the column and operate said column to effectively remove the water, the columns cost would exceed the financial benefit provided by the sulfolane recycle stream resulting from the column. This consequence occurs since nearly all water must be removed through the distillate in this column since any aqueous phase components caused our Aspen Hysys simulation to fail to converge on a solution. Since sulfolane and water make a corrosive mixture, eliminating the column also saved money by designing other equipment as carbon steel not exposed to this stream as opposed to the stainless steel material of construction that would be necessary if this stream were to be recycled. Our group suggests further studies be done on this failure to ensure that this innovation is of economic benefit. Sulfolane is recycled back to the sulfolane feed entering LLE-101 from 85% of the bottoms product of T-102 with the remaining 15% being purged. The flow rate of sulfolane being recycled back to the sulfolane feed stream equals 48,100 lb/hr for feed K and 46,300 lb/hr for feed TQ1. This saves the process $879 million and $845 million annually for the respective feed streams. Such a savings could be the difference between an economically favorable project as opposed to a profit loss under some tax regimes.

The extraction section entails two columns: T-102 and T-103. T-102 and T-103 have reboilers and T-103 has a condenser with a reflux drum. P-102 A/B is used to elevate pressure of the stream before entering T-103. P-103 A/B is used in the reflux system of T-103. Three more heat exchangers are used to cool feed entering LLE-101 and vapors leaving T-102. Table 5 lists the bare module cost for all equipment present in the process but a more specific list for the extraction section is depicted in Table 44.

Table 44: Bare Module Capital Cost – Extraction Section

Equipment	Cost
LLE -101	$2,040,000
LLE -102	$1,950,000
T - 102	$317,000
T - 103	$781,000
V - 103	$8,500
E - 105	$92,800
E - 106	$108,000
E - 107	$105,000
E - 108	$111,000
E - 109	$91,600
E - 110	$93,300
P - 102 A/B	$14,500
P - 103 A/B	$14,500

The designed condenser pressure set point allows for adequate separation and purities to be reached. This pressure and the standard pressure drop across each tray sets the pressure throughout the column. The components present throughout the column create temperature profiles across the trays. We optimized column conditions by varying the stage the feed entered into the column and theoretical stages of said column until present worth cost was minimized. Figures 11 and 12 depict the temperature profiles for stream K of each column. Stage 0 in Figure 12 is the condenser temperature of T-103 with the final stage in each figure representing the reboiler temperature.

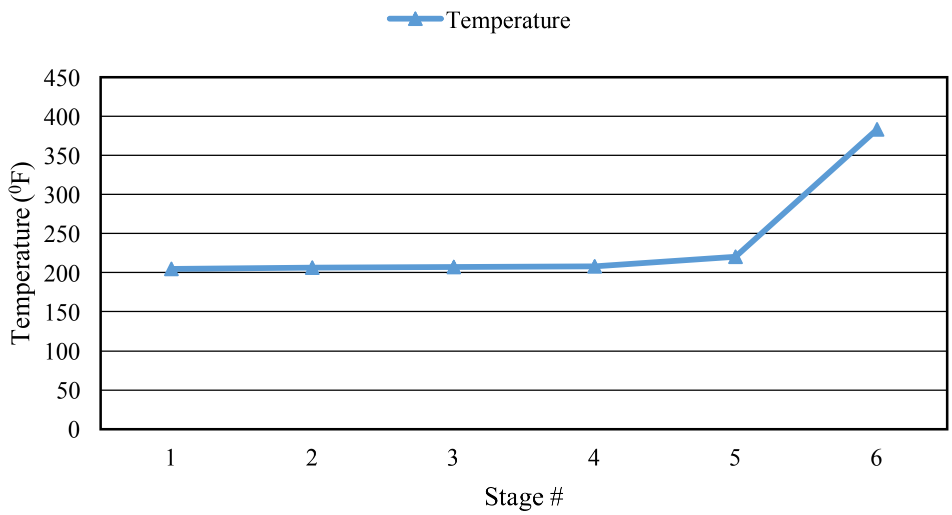


Figure 11: T-102 Temperature Profile for Stream K

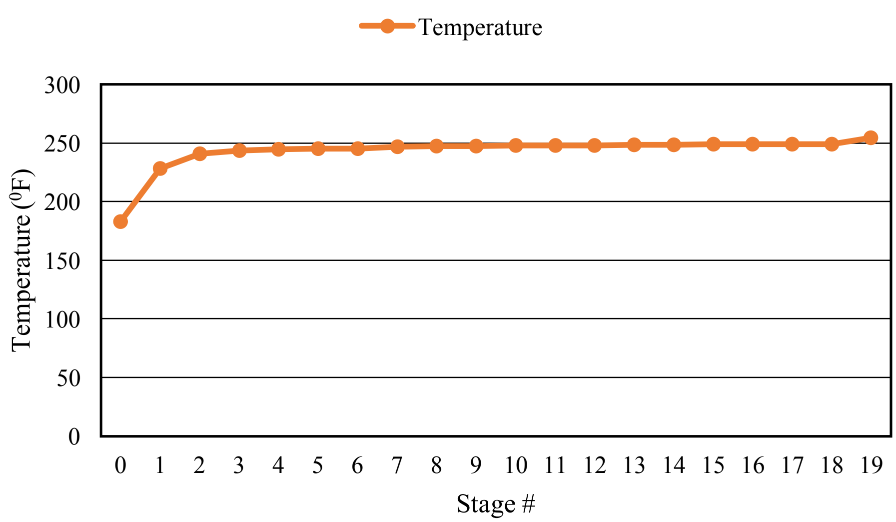


Figure 12: T-103 Temperature Profile for Stream K

In order to maintain these processing conditions, many utilities are necessary throughout the process equipment in this section. Tables 14-18 provide operating costs for each piece of equipment, but Table 45 itemizes the operating costs specific to the extraction section.

Table 45: Extraction Section Operating Costs for Stream K

Equipment	Cost
E - 105	$23,400
E - 106	$12,800
E - 107	$9,860
E - 108	$785,000
E - 109	$15,700
E - 110	$309,000
P - 102 A/B	$6,280
P - 103 A/B	$6,020
Labor	$86,600

Distillation

The following assumptions and constraints act as parameters for our distillation columns:

- the design assumes columns sized with 4 feet above the top tray to allow for vapor disengagement;
- the design assumes columns sized with 6 feet below the bottom tray to account for liquid level and reboiler return;
- columns are not sized above a height of 175 feet to avoid foundational problems or wind load concerns;
- the design assumes column trays to be two feet apart in the column [1];
- the design assumes columns possess a 0.1 psi drop per tray within the column [1];
- columns are sized using Fair's procedure [9];
- the design assumes tray efficiency to be 0.8 due to standard petrochemical trayed towers [10];
- the design assumes columns are fitted with sieve trays due to economic efficiency and high vapor flow rates [11], and
- benzene, toluene, and xylene product streams are designed to not fall below 99 mol% purity.

The primary goal of the distillation section is to separate the benzene, xylene, and toluene to 99 mol% in their respective product streams. The effort required in order to make those separations happen depends on the relative volatility between these respective components. Relative volatility is dependent upon temperature, pressure, and molecular properties of the components [9]. Relative volatility is measure by the quotient of two components K values which are derived from Henry's law in which the individual components vapor fraction is divided by its liquid fraction at a given temperature and pressure. The result of the division of one K value by the other gives a relative volatility between the two components. A relative volatility of 1 would be considered theoretically impossible to separate through distillation. Higher values indicate easier separations. Table 46 shows the distribution of relative volatilities between these three key components throughout the columns in the distillation section.

Table 46: Relative Volatilities in Distillation Section for Stream K

$\alpha_{A/B}$	Benzene/Toluene	Benzene/p-Xylene	Toluene/p-Xylene
T-104 Top (stage 1)	2.72	6.86	2.52
T-104 Bottom (stage 16)	2.25	4.96	2.20
T-105 Top (stage 1)	2.33	5.37	2.30
T-105 Bottom (stage 34)	2.05	3.98	1.94

As the table above shows, across many different column environments the two easiest components to separate are benzene and para-xylene. The toughest to separate are toluene and para-xylene; consequently, our group decided to use 34 theoretical stages in Aspen HYSYS to ensure 99 mol% purity for each.

As is also depicted in the table above, the distillation section entails two columns: T-104 and T-105. Both columns have condensers and reboilers associated with them, E-111-114. Both condensers have reflux drums upon their outlet to ensure for safe operating conditions to minimize damage to reflux pumps, P-104-105 A/B. Table 5 lists the bare module capital cost for all equipment present in this section, but it is also detailed here below in Table 47.

Table 47: Bare Module Capital Cost - Distillation Section

Equipment	Cost
T - 104	$1,390,000
T - 105	$917,000
V -104	$142,000
V -105	$148,000
E - 111	$96,900
E - 112	$116,000
E - 113	$182,000
E - 114	$118,000
P - 104 A/B	$11,900
P - 105 A/B	$12,300

The designed condenser pressure set point allows for adequate separation and purities to be reached. This pressure and the standard pressure drop across each tray sets the pressure throughout the column. The components present throughout the column create temperature profiles across the trays. We optimized column conditions by varying the stage the feed entered into the column and theoretical stages of said column until present worth cost was minimized. Figures 13 and 14 depict the temperature profiles for stream K of each column. Stage 0 in both figures is the condenser temperature with the final stage in each figure representing the reboiler temperature.

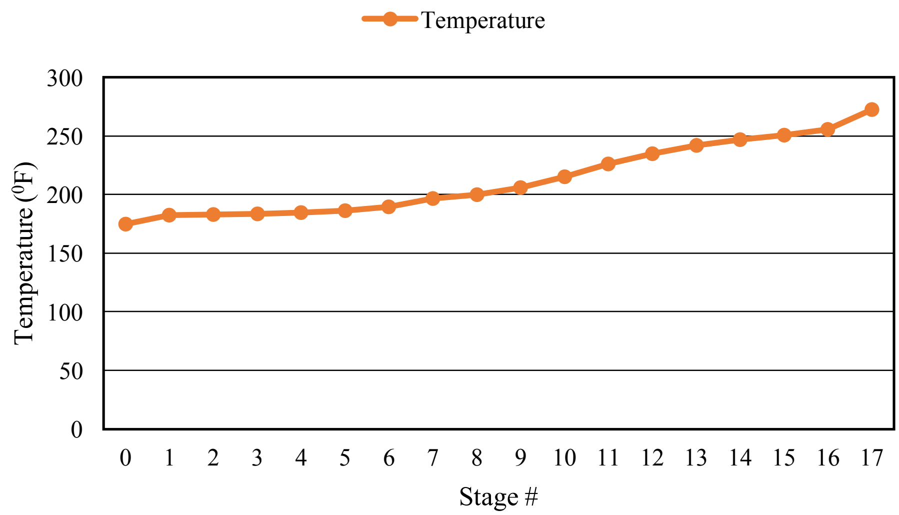


Figure 13: T-104 Temperature Profile for Stream K

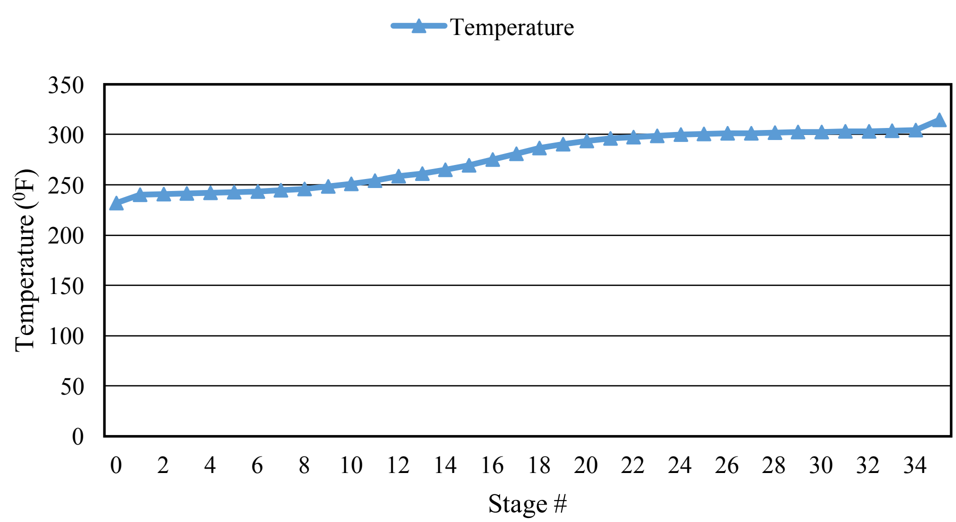


Figure 14: T-105 Temperature Profile for Stream K

In order to maintain these processing conditions, many utilities are necessary throughout the process equipment in this section. Tables 14-18 provide operating costs for each piece of equipment, but Table 48 itemizes the operating costs specific to the distillation section.

Table 48: Distillation Section Operating Costs for Stream K

Equipment	Cost
E - 111	$22,600
E - 112	$105,000
E - 113	$8,900
E - 114	$123,000
P - 104 A/B	$1,990
P - 105 A/B	$3,750
Labor	$52,000

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