Letter of Transmittal
To: Mr. Abbasi (COO)

From: Superior Engineering Construction and Procurement Firm (EPC)

Date: April 16th, 2021

Subject: Proposed Toppings Refinery Retrofit

Dear Mr. Abbasi,

Per your request, a preliminary analysis and retrofit of the toppings refinery was completed in order to adhere to the western refinery safety and production standards sought after by the Iraqi government. This design uses a fixed bed continuous catalytic reformer to process naphtha into product streams including benzene, toluene, and xylene. The process was evaluated with both the TQ1 and K feed streams. The toppings refinery was retrofitted with superior process safety, operational standards, and efficiency to eliminate the harboring of hazardous benzene and instead create a lucrative byproduct. The successful completion of this design is enclosed and outlined in a process description, process safety evaluation, and economic analysis.

For feed K, the anticipated capital cost of this refinery is $13,000,000. The estimated operational cost is $24,700,000 with a yearly product revenue of $272,800,000. For feed TQ1, the anticipated capital cost is $14,400,000. The predicted operation cost is $38,700,000 and yearly product revenue is $ 385,000,000. After the evaluation of all process economics and safety standards, both feed stream compositions are considered economically attractive.

Sincerely,
Your Superior EPC Team

AIChE
Student Design
Competition

April 16th, 2021

Executive Summary

To account for developing safety standards, the Iraqi government is striving to rehabilitate the larger producing refineries and cease operations in smaller, more hazardous refineries. The toppings refinery in Kirkuk, Iraq needs a retrofitted design modeled after western refining standards to replace the current hazardous benzene product stream with a stream in compliance with industry standards. The naphtha feedstock in both K and TQ1 compositions were evaluated in process design for economic feasibility.

The process follows a similar design as the base case process flow diagram provided. The naphtha feedstock flows into an extraction section which includes a fired heater with three fixed bed continuous catalytic reactors operating in series. This section removes hydrogen and the lighter hydrocarbons from the process stream. The benzene product of the reactors flows into a vapor feed separator before entering the extraction section. The extraction section consists of two liquid-liquid extractors, three stripping columns, and one distillation column to extract a blended stream of benzene, toluene, and xylene or BTX by removing other hydrocarbons. This reformate stream then flows into the distillation section to isolate the stream into the three product streams. This process also utilizes pumps, heat exchangers, column condensers, and reboilers to create the desired product streams.

Based on the economic analysis, the design is economically attractive with both feed stream compositions. For feed K, the anticipated capital cost of this refinery is $13,000,000. The estimated operational cost is $24,700,000 with a yearly product revenue of $272,800,000. The net present value is $467,034,757 in Kurdish and $353,689,661 in Iraq. For feed TQ1, the anticipated capital cost is $14,400,000. The predicted operation cost is $38,700,000 and yearly product revenue is $ 385,000,000. The net present value is $714,142,721 in Kurdish and $542,288,196 in Iraq. The design was depreciated over 10 years.

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Brief Process Description

The purpose of this design is to process the compound naphtha, a blend of hydrocarbons, into benzene, toluene, and xylene, or BTX. This process involves first an endothermic reaction section to produce benzene, an extraction section to isolate BTX, and lastly a distillation section to separate the reformate into benzene, toluene, and xylene. For this project, two crude unit feeds with different naphtha compositions called "K" and "TQ1" were used in process simulations (Table 1). Costing and Economic analysis was performed for both streams as well. Both naphtha feeds enter the process at 70°F and 1.2 bara and the refinery processes 35,000 barrels a day of crude oil. All process simulations were designed using Aspen HYSYS.

	TQ1	K
Naptha % Volume of Crude	28	20
Specific Gravity	0.7308	0.749
n-decane mole %	77.8	59.7
cyclohexane mole %	20.6	31.3
benzene mole %	1.6	9

Table 1: Crude Oil Feed Naphtha Compositions

The reaction section consists of three packed bed reactors in series as well as a fire heater to facilitate the endothermic reactions. The initial naphtha stream is pumped up to a higher pressure before entering the fire heater. Four different reactions take place within these reactors including cycloalkane dehydrogenation, cycloalkane cracking, alkane cracking, and cycloalkane cyclization. The purpose of these reactions is to convert naphtha cyclohexane, representing all feed hydrocarbons and cyclohexenes, into benzene, representing all aromatics. All reaction information including formulas and rate data was provided to the group in the problem statement. After the reactions are completed, the stream is then cooled and separated through a vapor feed separator with the vapor being recycled and the liquid being cooled again before continuing to the extraction section.

$$C_6H_{12} \rightarrow C_6H_6 + 3H_2$$

Cycloalkane Dehydrogenation

$$C_6H_{12} + 2H_2 \rightarrow 0.4C_5H_{12} + 0.4C_4H_{10} + 0.4C_3H_8 + 0.4C_2H_6 + 0.4CH_4$$

Cycloalkane Cracking

$$4.5C_{10}H_{22} + 4.5H_2 \rightarrow C_9H_{20} + C_8H_{18} + C_7H_{16} + C_6H_{14} + C_5H_{12} + C_4H_{10} + C_3H_8 + C_2H_6 + CH_4$$

Alkane Cracking

$$C_6H_{12} + H_2 \rightarrow C_6H_{14}$$

Cycloalkane Cyclization

The purpose of the extraction section is to isolate BTX from the process feed. For the purposes of the simulation the reformate "benzene," is separated to 99% purity after leaving the extraction section, however, this reformate is a mixture of benzene, toluene, and xylene. The compositions of these components are found using equations given to the group in the problem statement, and these new compositions are implemented into the process stream before it enters the distillation section.

The extraction section consists of three strippers, two liquid-liquid extractors, and a distillation column known as the major fractionator. The product stream first enters a stripper, T-100, where mostly light hydrocarbons are pulled out of the top of the stripper and purged, and the liquid product stream continues through the process. Most of the benzene in the product stream is separated into the bottom outlet of the first liquid-liquid extractor, T-102, where it enters the third stripper. The top outlet of T-102 contains mostly linear alkanes, which are extracted in the second liquid-liquid extractor, T-103 using water. The stream of linear alkanes is used as fuel and can be sold and calculates into the overall profits of the refinery. The water is entered into stripper 2, T-104, along with a slight amount of sulfolane, where it is purged in the overhead and the sulfolane is recycled into the first liquid-liquid extractor. Stripper 3, T-105, extracts mostly pure benzene from the top outlet of T-100. The bottoms product of this tower, sulfolane is mixed with the stripper 2 bottoms and recycled. Within this recycle stream, pure sulfolane is introduced, this product acts as a solvent in the extraction process of T-100, and the purpose of recycling the solvent from the strippers is to lower the initial costs of using sulfolane, as well as to lessen the amount of waste. Lastly, T-106, or the major defractionator separates reformate benzene to 99% purity in the distillate. The bottoms product of the distillation column is recycled into the beginning of the extraction process.

The last section of the overall process is the distillation section. This section consists of two full distillation columns that separate the reformate stream, into pure benzene, toluene, and xylene. As said before the composition of this reformate mixture is calculated using equations given in the problem statement before it enters the distillation section. The first distillation column, T-107 separates purified benzene in the overhead from the toluene and xylene mixture. This mixture enters the second distillation column, T-108 from the bottoms of the fist column. This column separates toluene, through the overhead, and xylene, through the bottoms, to 99% purity. The block diagram and process flow diagrams for each specific section are shown below in Figures 1-4 and stream data has been added to highlight composition, temperature, pressure, and flowrate in Tables 2-4 below.

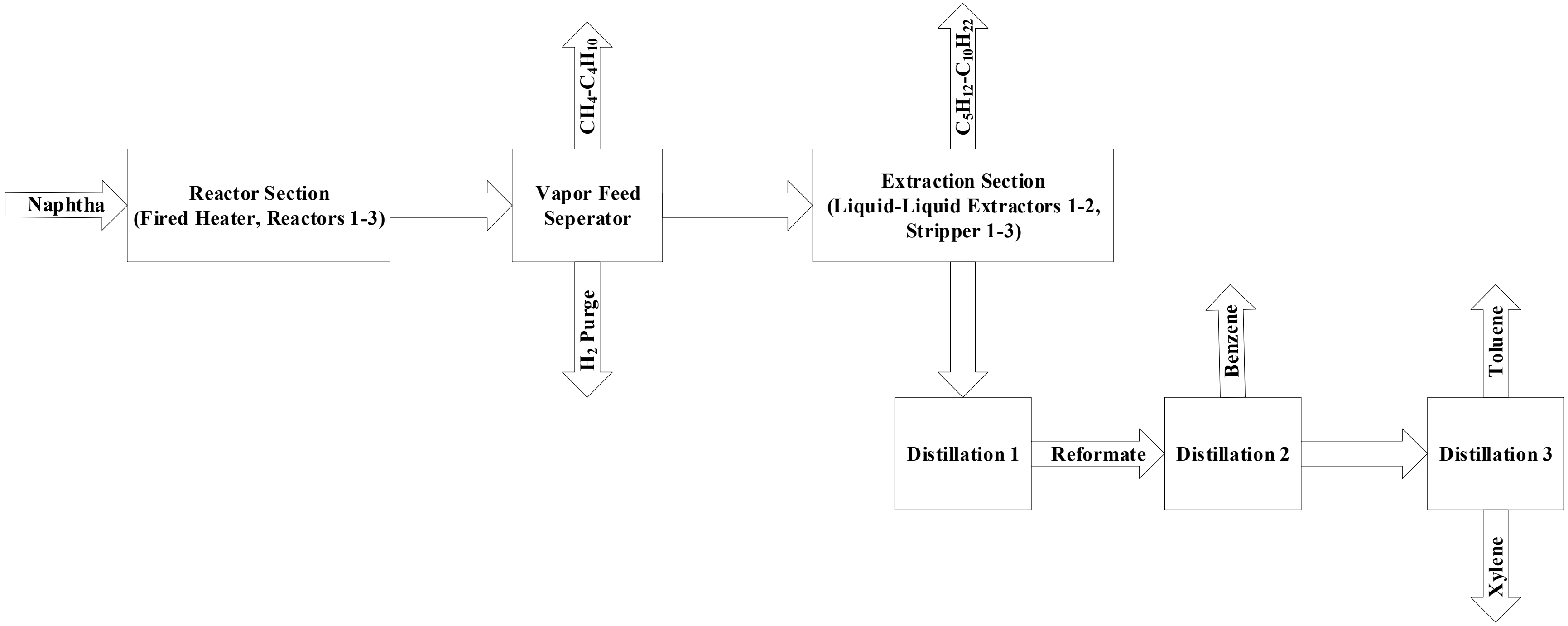

Figure 1: Block Flow Diagram

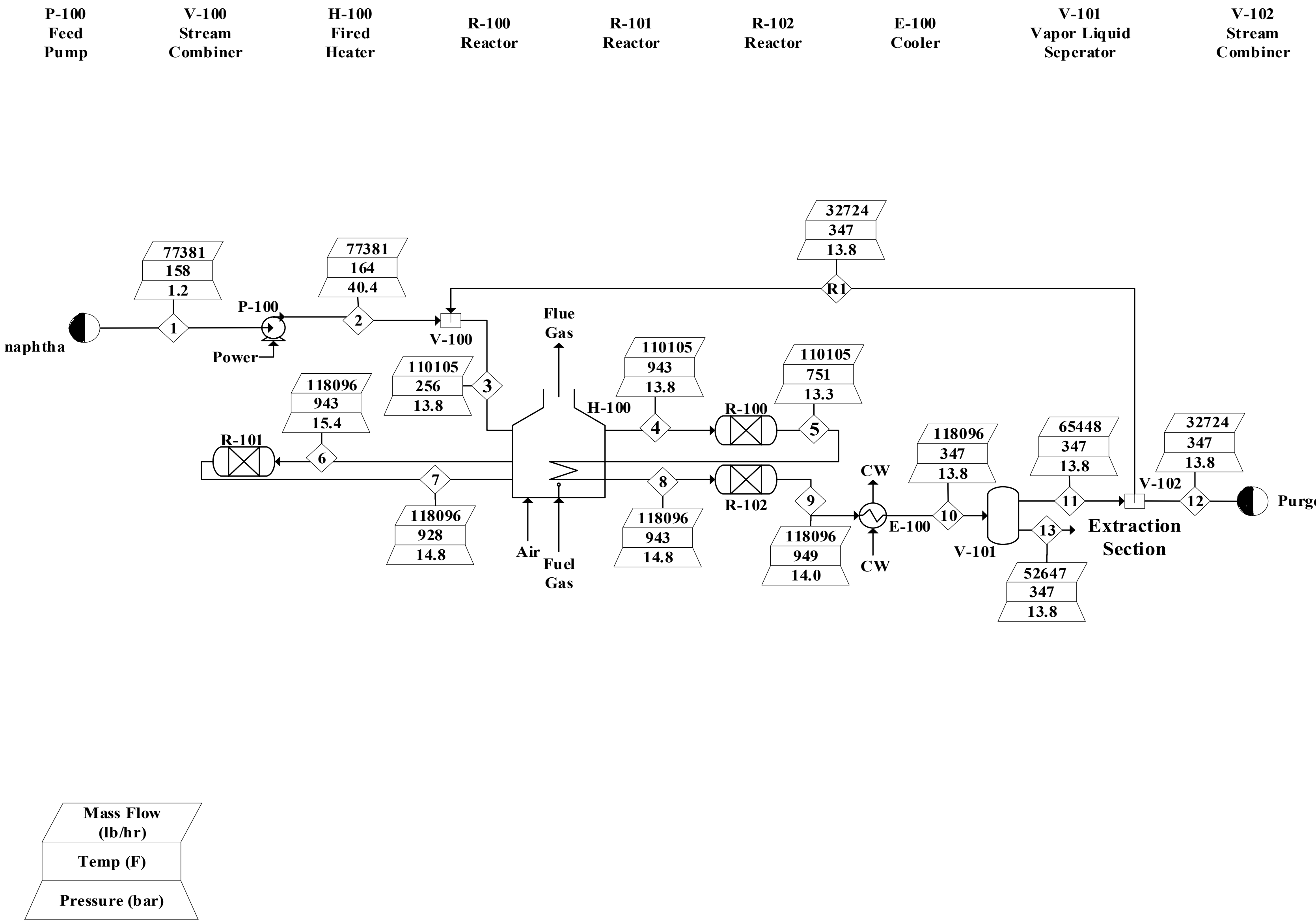

Figure 2: Reactor Process Flow Diagram for Feed K

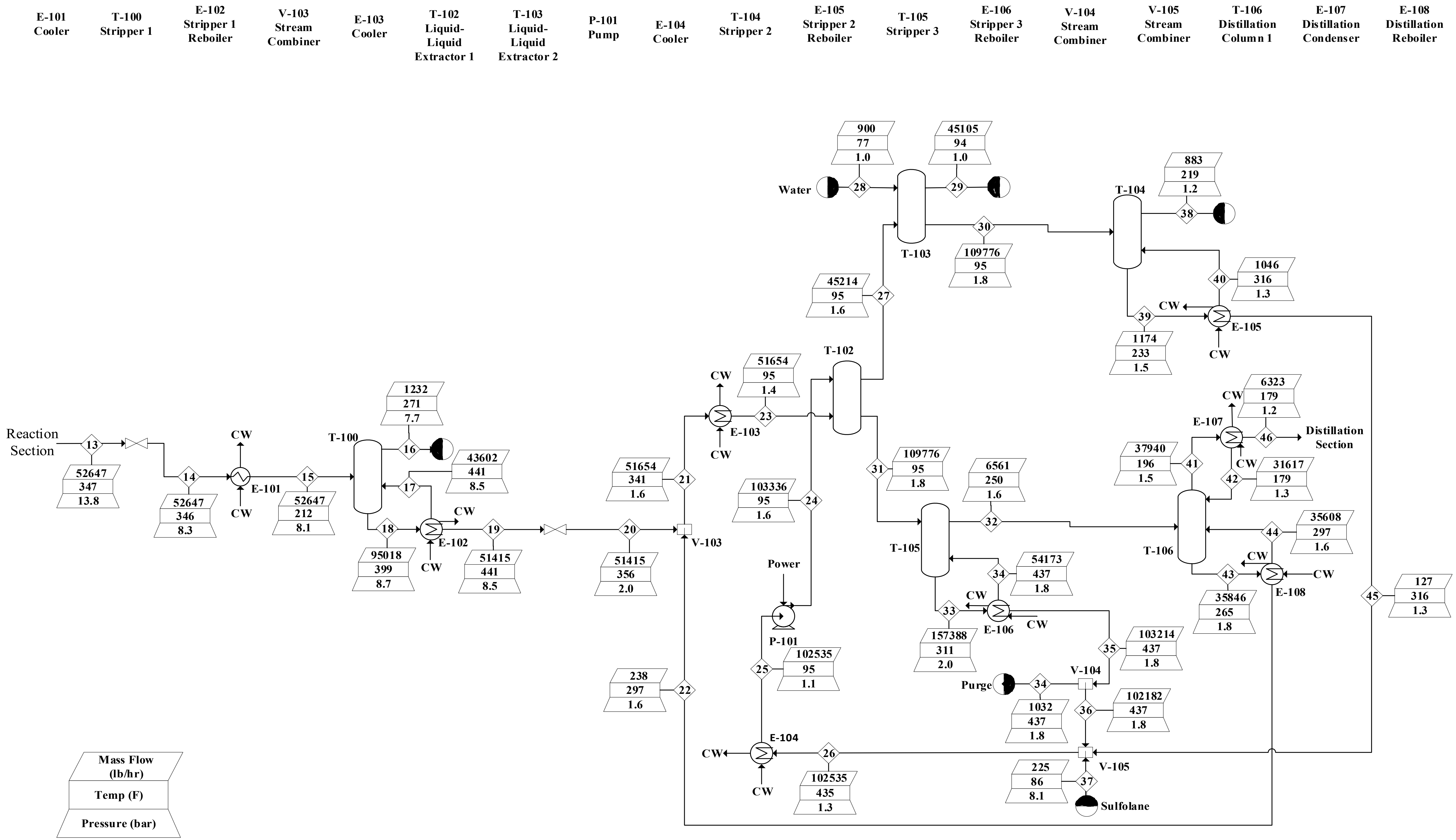

Figure 3: Extraction Process Flow Diagram for Feed K

P-102 Pump	E-113 Cooler	T-107 Distillation Column 2	E-109 Distillation 2 Condenser	E-110 Distillation 2 Reboiler	T-108 Distillation Column 3	E-111 Distillation 3 Condenser	E-112 Distillation 3 Reboiler

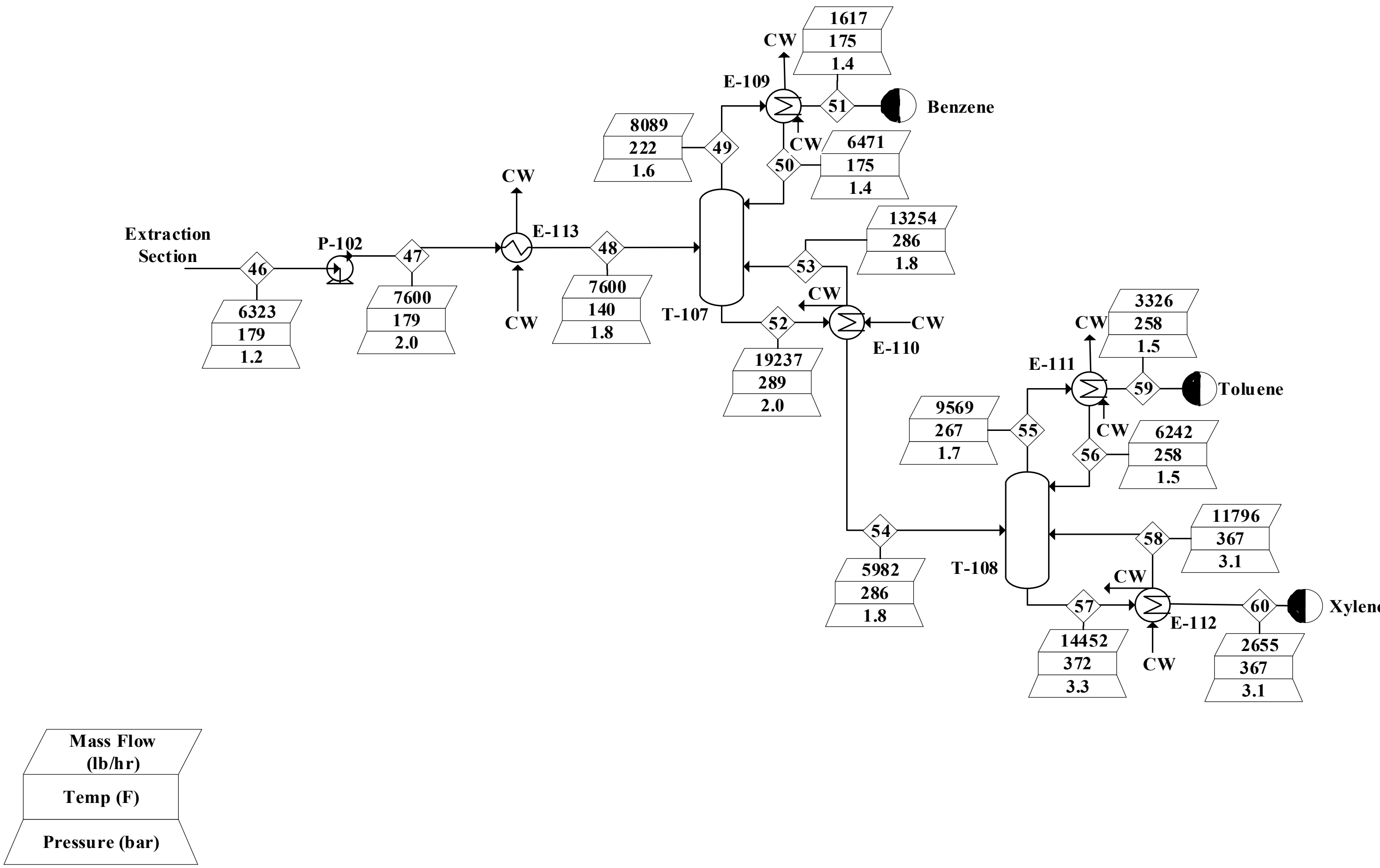

Figure 4: Distillation Process Flow Diagram for Feed K

Stream Number	1	2	3	R1	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Stream Label	Naphtha Inlet	Pumped Naphtha	Fired Heater Inlet	Separator Recycle	Reactor 1 Inlet	Reactor 1 Outlet	Reactor 2 Inlet	Reactor 2 Outlet	Reactor 3 Inlet	Reactor 3 Outlet	E-100 Outlet	V-101 Top Product	V-102 Purge	V-101 Bottom Product	E-101 Inlet	Stripper 1 Inlet	Stripper 1 Top Product	Stripper 1 Boil up	E-102 Inlet	E-102 Outlet	V-103 Inlet
Phase	Liq	Liq	AQ	AQ	Vap	AQ	Vap	AQ	Vap	AQ	AQ	AQ	AQ	AQ	AQ	AQ	Vap	Vap	AQ	AQ	AQ
Pressure (Bar)	1.2	40.4	13.8	13.8	13.8	13.3	15.4	14.8	14.8	14.0	13.8	13.8	13.8	13.8	8.3	8.1	7.7	8.5	8.7	8.5	2.0
Temperature (F)	158.0	163.9	256.4	347.0	943.0	751.1	943.0	927.7	943.0	949.2	347.0	347.0	347.0	347.0	345.5	212.0	271.3	441.0	399.3	441.0	356.0
Total Molar Flow (lbmole/hr)	654	654	1702	1048	1702	2210	2457	2526	2526	2532	2532	2096	1048	436	436	436	25	445	856	412	412
n-Decane	0.60	0.60	0.26	0.05	0.26	0.20	0.18	0.16	0.16	0.15	0.15	0.05	0.05	0.65	0.65	0.65	0.48	0.27	0.47	0.69	0.69
Cyclohexane	0.31	0.31	0.12	0.00	0.12	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.09	0.09	0.14	0.16	0.14	0.18	0.17	0.18	0.18	0.18	0.18	0.16	0.16	0.24	0.24	0.24	3.25	0.64	0.45	0.24	0.24
Hydrogen	0.00	0.00	0.35	0.57	0.35	0.50	0.48	0.48	0.48	0.47	0.47	0.57	0.57	0.01	0.01	0.01	4.77	0.00	0.00	0.00	0.00
Methane	0.00	0.00	0.03	0.05	0.03	0.02	0.03	0.04	0.04	0.04	0.04	0.05	0.05	0.00	0.00	0.00	1.02	0.00	0.00	0.00	0.00
Ethane	0.00	0.00	0.03	0.04	0.03	0.02	0.03	0.03	0.03	0.04	0.04	0.04	0.04	0.01	0.01	0.01	2.33	0.00	0.00	0.00	0.00
Propane	0.00	0.00	0.03	0.05	0.03	0.02	0.03	0.04	0.04	0.04	0.04	0.05	0.05	0.00	0.00	0.00	1.80	0.00	0.00	0.00	0.00
n-Butane	0.00	0.00	0.02	0.04	0.02	0.02	0.03	0.03	0.03	0.03	0.03	0.04	0.04	0.01	0.01	0.01	4.03	0.00	0.00	0.00	0.00
n-Pentane	0.00	0.00	0.02	0.03	0.02	0.01	0.02	0.02	0.02	0.03	0.03	0.03	0.03	0.02	0.02	0.02	6.56	0.01	0.00	0.00	0.00
n-Hexane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.04	0.01	0.00	0.00	0.00
n-Heptane	0.00	0.00	0.01	0.01	0.01	0.00	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.02	0.02	0.02	0.12	0.03	0.03	0.02	0.02
n-Octane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.00	0.00	0.02	0.02	0.02	0.06	0.02	0.02	0.02	0.02
n-Nonane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.02	0.02	0.02	0.03	0.01	0.02	0.02	0.02
Toluene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
p-Xylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SULFOLANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Air	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow (lb/hr)	77381	77381	110106	32724	110106	110106	118097	118097	118097	118097	118097	65449	32724	52648	52648	52648	1233	43603	95018	51415	51415
Volumetric Flow Rate (barrel/day)	7457	7440	148825	193257	545790	637695	705959	750785	759042	803504	392443	386513	193257	5930	8483	5963	7393	149605	10965	6349	278743

Table 2: Process Stream 1-20

Stream Number	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40
Stream Label	E-103 Inlet	T-106 Bottom Product	E-103 Outlet	P-101 Outlet	P-101 Inlet	E-104 Inlet	T-103 Inlet	Water	T-103 Top Outlet	T-103 Bottom Outlet	T-102 Bottom Outlet	T-105 Distillate	T-105 To Reboiler	T-105 Purge	T-104 Bottoms	T-104 Recycle	Sulfolan e	T-104 Distillate	T-104 To Reboiler	T-104 Reboiler Boilup
Phase	AQ	Liq	Liq	Liq	Liq	AQ	Liq	AQ	Liq	AQ	Liq	Vap	Liq	Liq	Liq	Liq	Liq	Vap	Liq	Vap
Pressure (Bar)	1.6	1.6	1.4	1.6	1.1	1.3	1.6	1.0	1.0	1.2	1.8	1.6	2.0	1.8	1.8	1.8	8.1	1.2	1.5	1.3
Temperature (F)	341.3	297.2	95.0	95.1	95.0	434.6	95.1	77.0	94.4	95.1	95.0	250.3	310.5	437.0	437.0	437.0	86.0	219.3	233.1	316.3
Total Molar Flow (lbmole/hr)	414	2	414	861	861	861	332	50	332	50	950	83	1359	9	867	858	2	49	54	53
n-Decane	0.69	0.43	0.69	0.00	0.00	0.00	284.98	0.00	0.86	0.00	0.00	0.01	0.15	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cyclohexane	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	0.24	0.04	0.24	0.03	0.03	0.03	18.52	0.00	0.06	0.00	0.11	0.98	0.18	0.03	0.03	0.03	0.00	0.00	0.00	0.00
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Butane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Pentane	0.00	0.00	0.00	0.00	0.00	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Hexane	0.00	0.00	0.00	0.00	0.00	0.00	0.63	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Heptane	0.02	0.19	0.02	0.00	0.00	0.00	7.61	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Octane	0.02	0.18	0.02	0.00	0.00	0.00	8.82	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Nonane	0.02	0.08	0.02	0.00	0.00	0.00	9.71	0.00	0.03	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Toluene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
p-Xylene	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SULFOLANE	0.00	0.08	0.00	0.97	0.97	0.97	1.05	0.00	0.00	0.02	0.88	0.00	0.66	0.97	0.97	0.97	1.00	0.00	0.04	0.02
H2O	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.98	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.96	0.98
Air	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow (lb/hr)	51655	239	51655	102536	102536	102536	45215	901	45105	1010	109777	6562	157388	1032	103215	102183	225	883	1174	1047
Volumetric Flow Rate (barrel/day)	392574	26	4748	5688	5688	20165	4271	61	4265	67	6231	115440	11284	67	6664	6598	12	91413	82	102856

Table 3: Process Stream 21-40

Stream Number	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
Stream Label	T-106 To Condenser	T-106 Condenser Reflux	T-106 To Reboiler	T-106 Reboiler Boilup	T-104 Bottoms	BTX Reformate	Pumped BTX Inlet	Cooled BTX Inlet	T-107 To Condenser	T-107 Condenser Reflux	Benzene	T-107 To Reboiler	T-107 Reboiler Boilup	T-107 Bottoms	T-108 To Condenser	T-108 Condenser Reflux	T-108 To Reboiler	T-108 Reboiler Boilup	Toluene	Xylene
Phase	Vap	Liq	Liq	Vap	Liq	Liq	Liq	Liq	Vap	Liq	Liq	Liq	Vap	Liq	Vap	Liq	Liq	Vap	Liq	Liq
Pressure (Bar)	1.5	1.2	1.8	1.6	1.3	1.2	2.0	1.8	1.6	1.4	1.4	2.0	1.8	1.8	1.7	1.5	3.3	3.1	1.5	3.1
Temperature (F)	195.5	178.6	265.3	297.2	316.3	178.6	178.7	140.0	222.4	174.6	174.6	289.1	286.0	286.0	267.0	257.5	372.1	367.0	257.5	367.0
Total Molar Flow (lbmole/hr)	486	405	328	327	1	81	81	81	100	80	20	200	139	61	104	68	136	111	36	25
n-Decane	0.00	0.00	0.14	0.14	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Cyclohexane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Benzene	1.00	1.00	0.10	0.10	0.00	0.18	0.18	0.18	0.75	0.75	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hydrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Ethane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Butane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Pentane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Hexane	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Heptane	0.00	0.00	0.46	0.46	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Octane	0.00	0.00	0.21	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
n-Nonane	0.00	0.00	0.05	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Toluene	0.00	0.00	0.00	0.00	0.00	0.50	0.50	0.50	0.24	0.24	0.24	0.70	0.75	0.59	0.99	0.99	0.02	0.02	0.99	0.01
p-Xylene	0.00	0.00	0.00	0.00	0.00	0.31	0.31	0.31	0.00	0.00	0.00	0.30	0.25	0.41	0.01	0.01	0.98	0.98	0.01	0.99
SULFOLANE	0.00	0.00	0.03	0.03	0.89	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2O	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Air	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Oxygen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow (lb/hr)	37941	31617	35846	35608	127	7600	7600	7600	8089	6472	1618	19237	13255	5982	9569	6242	14452	11800	3327	2656
Volumetric Flow Rate (barrel/day)	693663	2676	3921	498287	8	642	642	625	133357	546	136	1764	185027	547	139620	559	1418	93870	298	259

Table 4: Process Streams 41-60

Economic Analysis and Sensitivities

Capital Cost Estimates

The costs associated with the installation of all equipment designed for Mr. Abbasi's plant were estimated via Appendix A of Analysis, Synthesis, and Design of Chemical Processes. The group analyzed two separate versions of the simulation; one simulation regarding the TQ1 Feed listed as version 1.99, and the other regarding the K Feed listed as version 2.2. The costs calculated and variables in Appendix A for both simulations were based on 2001 prices and then escalated to 2021 standards using the Chemical Engineering Plant Cost Index. The CEPCI values for 2001 and 2021 are 397 and 617, respectively[1]. All installation, maintenance, and operating costs are based on current 2021 dollars.

Both simulations were also evaluated effectively towards both Iraqi and Kurdish taxes to utilize the difference in bracketing for each form of government. Once those analyses were formulated, a sensitivity analysis for both tax laws were carried out to analyze a difference of external factors. The analyses also will show which factors affect the Net Positive Value of the project and Rate of Return accordingly.

Contingencies and fees were accounted for in the Total Fixed Capital Cost. From information regarding contingency and fees in Analysis, Synthesis, and Design of Chemical Processes, the contingency rate and fees were assumed to be 15% and 3%, respectively. These values were then utilized in the expense template as working capital and added to the set capital cost. The method used to calculate the total fixed capital cost was a summation of all sized equipment that would be purchased in the year 2021 and installed in the year 2022. After all installation, sizing, and variables were calculated, the total fixed capital cost for each simulation came out to be approximately $16,600,000 and $15,000,000. Tables 5 and 6 showcase the specific apparatus cost for each process unit in both the TQ1 feed and K feed, respectively.

The more significant portion of the total capital cost will go towards reactors, heat exchangers, and the fired heater. The fired heater is the largest initial cost and has the highest utility cost per unit. Pumps, drums, and the vapor feed separator will contribute to the lower portion of the total cost.

Equipment Costing Overview TQ1 Feed			
Section	**Description**	**PFD Label**	**Equipment Today's Cost**
Heater/Furnace	Fired Heater (K Feed)	H-100	$4,615,005
Reactors	Reactor I	R-100	$ 844,882
	Reactor II	R-102	$ 866,185
	Reactor II	R-103	$ 866,185
Process Vessel	Stripper I	T-100	$ 273,785
	Stripper II	T-105	$ 75,018
	Stripper III	T-104	$ 586,497
	Column I	T-106	$ 152,731
	Column II	T-107	$ 106,810
	Column III	T-108	$ 577,560
	Liquid Extractor I	T-102	$ 205,757
	Liquid Extractor II	T-103	$ 287,725
Condensers	Column I Condenser	E-107	$ 113,217
	Column II Condenser	E-109	$ 72,466
	Column III Condenser	E-111	$ 129,284
Reboilers	Stripper I Reboiler	E-102	$ 207,660
	Stripper II Reboiler	E-106	$ 130,447

	Stripper III Reboiler	E-105	$ 236,438
	Column I Reboiler	E-108	$ 185,918
	Column II Reboiler	E-110	$ 134,782
	Column III Reboiler	E-112	$ 204,950
Pumps	Naphtha A/B	P-100	$ 372,968
	P-101 A/B	P-101	$ 26,464
	BTX A/B	P-102	$ 27,976
	Stripper I Reboiler A/B	N/A	$ 75,661
	Stripper II Reboiler A/B	N/A	$ 100,929
	Stripper III Reboiler A/B	N/A	$ 91,284
	Column I Reboiler A/B	N/A	$ 47,051
	Column II Reboiler A/B	N/A	$ 36,441
	Column III Reboiler A/B	N/A	$ 50,149
	Column I Condenser A/B	N/A	$ 33,426
	Column II Condenser A/B	N/A	$ 43,317
	Column III Condenser A/B	N/A	$ 35,969
Reflux Drums	Column I Condenser Drum	N/A	$ 55,688
	Column II Condenser Drum	N/A	$ 15,260
	Column III Condenser Drum	N/A	$ 189,000
Heat Exchangers	Cooler I	E-100	$ 451,256

	Cooler II	E-101	$ 201,922
	Cooler III	E-102	$ 424,941
	Cooler IV	E-103	$ 685,121
	Cooler V	E-104	$ 118,399
Separators	Vapor Feed Separator	V-101	$ 472,921
Total Equipment Costs			**$ 14,429,448**

Table 5: Equipment Costing Overview TQ1 Feed

Equipment Costing Overview K Feed			
Section	**Description**	**PFD Label**	**Equipment Today's Cost**
Heater/Furnace	Fired Heater (K Feed)	H-100	$ 4,300,577
Reactors/Catalyst	Reactor I	R-100	$ 844,882
	Reactor II	R-102	$ 866,185
	Reactor II	R-103	$ 866,185
Process Vessel	Stripper I	T-100	$ 273,785
	Stripper II	T-105	$ 75,018
	Stripper III	T-104	$ 586,497
	Column I	T-106	$ 152,731
	Column II	T-107	$ 98,405
	Column III	T-108	$ 317,523

	Liquid Extractor I	T-102	$ 243,916
	Liquid Extractor II	T-103	$ 287,725
Condensers	Column I Condenser	E-107	$ 104,053
	Column II Condenser	E-109	$ 73,251
	Column III Condenser	E-111	$ 99,427
Reboilers	Stripper I Reboiler	E-102	$ 209,908
	Stripper II Reboiler	E-106	$ 135,677
	Stripper III Reboiler	E-105	$ 214,773
	Column I Reboiler	E-108	$ 171,742
	Column II Reboiler	E-110	$ 138,174
	Column III Reboiler	E-112	$ 199,258
Pumps	Naphtha A/B	P-100	$ 309,072
	P-101 A/B	P-101	$ 23,935
	BTX A/B	P-102	$ 28,920
	Stripper I Reboiler A/B	N/A	$ 71,196
	Stripper II Reboiler A/B	N/A	$ 144,327
	Stripper III Reboiler A/B	N/A	$ 59,122
	Column I Reboiler A/B	N/A	$ 80,585
	Column II Reboiler A/B	N/A	$ 36,590

	Column III Reboiler A/B	N/A	$ 45,774
	Column I Condenser A/B	N/A	$ 33,484
	Column II Condenser A/B	N/A	$ 41,109
	Column III Condenser A/B	N/A	$ 35,643
Reflux Drums	Column I Condenser Drum	N/A	$ 54,222
	Column II Condenser Drum	N/A	$ 20,289
	Column III Condenser Drum	N/A	$ 19,977
Heat Exchangers	Cooler I	E-100	$ 384,031
	Cooler II	E-101	$ 171,216
	Cooler III	E-102	$ 206,876
	Cooler IV	E-103	$ 387,899
	Cooler V	E-104	$ 123,346
Separators	Vapor Feed Separator	V-101	$ 508,549
Total Equipment Cost			**$ 13,045,851**

Table 6: Equipment Costing Overview K Feed

Revenue and Operating Estimates

In order for the team to perform an economic analysis and determine the profitability of Mr. Abbasi's plant, the yearly revenue of the plant and total operating expenses were calculated. For the project's revenue, Benzene, Toluene, P-Xylene, Diesel, and Gasoline flow rates were taken from the Aspen HYSYS simulation and revenues were evaluated. Each product was given a different selling price provided in the project statement. Once the revenue for each product was determined, the total yearly revenue was summed from each product with a service factor of

91%. The total yearly revenue for the plant was determined to be $272,806,869. The total yearly revenue based on each component's sales is shown below in Table 7.

Yearly Revenue K Feed (Full Operating Year Basis and 91% Service Factor)			
Component	**Sales Price**	**Yearly Production**	**Yearly Revenue**
Benzene	$ 3.29 / gal	1,884,057 gal / yr	$ 5,260,287
Toluene	$ 2.792 / gal	3,907,617 gal / yr	$ 10,910,067
P-Xylene	$ 2.792 / gal	3,142,650 gal / yr	$ 8,774,279
Diesel	$ 0.98 / L	247,507,670 L / yr	$ 242,557,517
Gasoline	$ 0.63 / L	8,420,190 L / yr	$ 5,304,720
Total Yearly Revenue			**$ 272,806,869**

Table 7: Yearly Revenue K Feed (Full Operating year Basis and 91% Service Factor)

Yearly Revenue TQ1 (Full Operating Year Basis and 91% Service Factor)			
Component	**Sales Price**	**Yearly Production**	**Yearly Revenue**
Benzene	$ 3.29 / gal	1,712,361 gal / yr	$ 4,780,912
Toluene	$ 2.792 / gal	5,255,124 gal / yr	$ 14,672,306
P-Xylene	$ 2.792 / gal	3,751,251 gal / yr	$ 10,473,493
Diesel	$ 0.98 / L	333,458,887 L / yr	$ 326,789,709
Gasoline	$ 0.63 / L	45,019,872 L / yr	$ 28,362,519
Total Yearly Revenue			**$ 385,078,939**

Table 8: yearly Revenue TQ1 Feed (Full Operating Year Basis and 91% Service Factor)

In order to determine the total annual costs associated with Mr. Abbasi's plant, utility and operating costs were calculated. Cooling water, pressurized steam, and natural gas inlets were all used as utilities within the process. Pricing for all of these were given in the problem statement.

For the reaction section, reactor maintenance, pump operation, and heater natural gas supply rates were all estimated. Initially, the Naphtha pump was costed to accommodate the larger amount of Naphtha feed that is needed for the process. Electricity in the form of kW-h was then brought to the annual estimation of power consumed. For the reactors, jacket operation and catalyst costs were calculated to accommodate the reactors. The jacket was sized and costed to be operated for a period of 8 weeks after a period of 9 years. This value is an estimate and not a strict regulation. For the catalyst, the team found that the catalyst will last a total of 5 years before needing to be replaced or refilled. For the fired heater, the natural gas inlet rate was determined and cost via rates of MMBTU/hr. The total annual operating cost for the reaction section came out to be approximately $4,500,000, the highest costing section of the process.

For the extraction section, pressurized steam, cooling water, electricity, and water inlets were estimated. For the towers, diverging between strippers, distillation columns, and liquid extractors make up most of this section. Each stripper was manufactured with a reboiler and adjacent pump. The distillation columns each fitted with a condenser, reboiler, reflux drum, and adjacent pumps to their polar units were all analyzed. Finally, the liquid extractors were formatted without any of the previous attachments, but still required water inlets that were evaluated. Each condenser and reboiler was costed separately to accommodate the differing flow rates for each unit, and operating costs were determined as follows. Reboilers and condensers were modeled as heat exchangers with suggestions from Analysis, Synthesis, and Design of Chemical Processes. The reboilers were sized with their pressurized steam flow rates at units of kg/year. The condensers were sized with their cooling water flow rates at units of GJ/year. The condensers were also sized with reflux drums and pumps to push distillate to the next part of the process. The total annual operating cost for the extraction section came out to be approximately $2,420,000, the second highest costing section of the process despite having the most units.

Finally, for the distillation section, the distillation columns, BTX pump, and coolers were evaluated. The BTX pump was modeled to determine the kW-h per year consumed. The cooler was modeled to determine the cooling water flow rate and cost via units of GJ/year. The two distillation columns that give the final products of Benzene, Toluene, and P-Xylene were sized with the same method as the previous towers. Condensers, reflux drums, reboilers, and pumps were modeled to cost these towers. The total annual operating cost for the distillation section came out to be approximately $850,000, the lowest costing section of the process. The total cost for utilities associated with the process for the K feed is shown below in Table 8.

Yearly Operating/Utility Costs K Feed (Full Operating Year Basis and 91% Service Factor)	
Section	**Annual Operating Cost**
Reaction Section	$ 4,458,021
Extraction Section	$ 2,416,342
Distillation Section	$ 851,107
Total Operating/Utility Cost	**$ 7,725,266**

Table 9: Yearly Operating/Utility Costs for K Feed (Full Operating Year Basis and 91% Service Factor)

Yearly Operating/Utility Costs TQ1 Feed (Full Operating Year Basis and 91% Service Factor)	
Section	**Annual Operating Cost**
Reaction Section	$ 5,803,808
Extraction Section	$ 4,075,162
Distillation Section	$ 1,954,600
Total Operating/Utility Cost	**$ 11,833,570**

Table 10: Yearly Operating/Utility Costs for TQ1 Feed (Full Operating Year Basis and 91% Service Factor)

Cash Flow and Economic Analysis

Cash flow tables were determined for each naphtha feed stream to determine the economics involved in designing the new refinery. Cash flow analysis was performed for each stream twice, each under Iraqi and Kurdish taxes. In Iraq, a tax rate of 35% was used while a tax rate of 15% was used in Kurdish. A 30-year project evaluation was performed for each stream in both locations, and a hurdle rate of 15% was used for all economic analyses. The fixed capital was depreciated using the 10-year MACRS depreciation scale for refineries.

For economic analysis purposes, all fixed capital was shown to be purchased in 2021, while production within the refinery is planned to start in September 2023, based on the timing of religious holidays that occur over the summer. Fixed capital depreciation begins in 2023 as well, based on the beginning of production.

To gain a full understanding of the economics associated with both naphtha process streams and different tax rates, the Net Present Value (NPV) of each stream in each country was calculated. These values are shown below in Table 9. Because the NPVs are all positive and fairly high this indicates economic attractiveness for both naphtha streams in both Iraq and Kurdish. The DCFROR values and the benefit cost ratios for both streams and locations are shown below in Table 9 as well. Because the DCFROR in all four cases is above the hurdle rate of 15%, and because the benefit cost ratio for all cases is positive, these values also indicate the economic attractiveness of the project.

Although it was stated before starting this project that feed K was of greater interest, economic analysis showed that feed TQ1 was more economically attractive in both Iraq and Kurdish. Despite this, feed K is still a feasible option for the refinery based on calculated economic parameters. The payback periods for each feed and location are also shown below and was calculated to be between 2 and 3 years in all four analyses.

Stream	K		TQ1	
Location	Iraq	Kurdish	Iraq	Kurdish
Net Present Value (NPV)	$351,325,878	$463,943,656	$539,924,412	$711,051,619
DCFROR	99%	117%	120%	140%
Benefit Cost Ratio (BCR)	9.36	12.20	12.84	16.74
Payback Period (years)	2.844	2.490	2.614	2.471

Table 11: Economic Parameters for Feeds K and TQ1

Sensitivity Analyses

When performing an economic analysis, risks and fluctuations are taken into account to analyze variations in the sizing of equipment, estimating labor, manufacturing costs, product production rates, labor costs, environmental utility effects, and reactant procurement cost. Each of these aspects change with respect to time and other developments in technology, so values and estimations of cost can be marginalized through a sensitivity analysis. The sensitivity analyses performed were selected for the factors that the team deemed to be the most influential in project life ROR and NPV.

To begin the analysis, the values that were chosen are listed in order of importance: capital cost, operating cost, and product revenue. These values were manipulated via a ∓20%

basis on both Iraqi and Kurdish standards. The decision to use a 20% variation to the variables was chosen to show the biggest impacts of risks and change. A loss or gain of 20% is a significant margin to show large fluctuations in the three categories surveyed. To keep consistency, only one variable was manipulated at a time while keeping the other aspects of the analysis unchanged to account for the impact of the altered variable. From the Figures 5-12 listed below, it can be found that the variable with highest impact on ROR and NPV is product revenue.

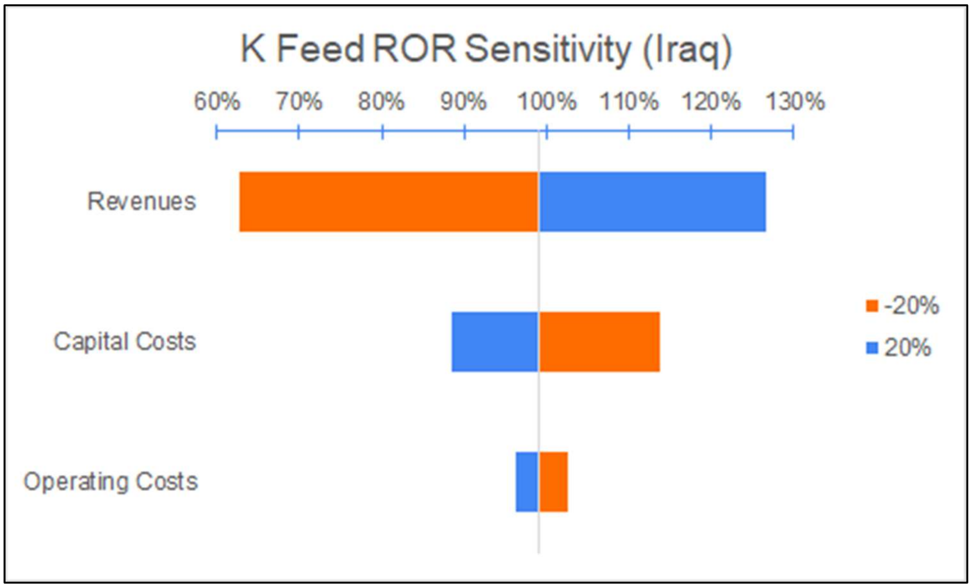

Figure 5: K Feed ROR Sensitivity (Iraq)

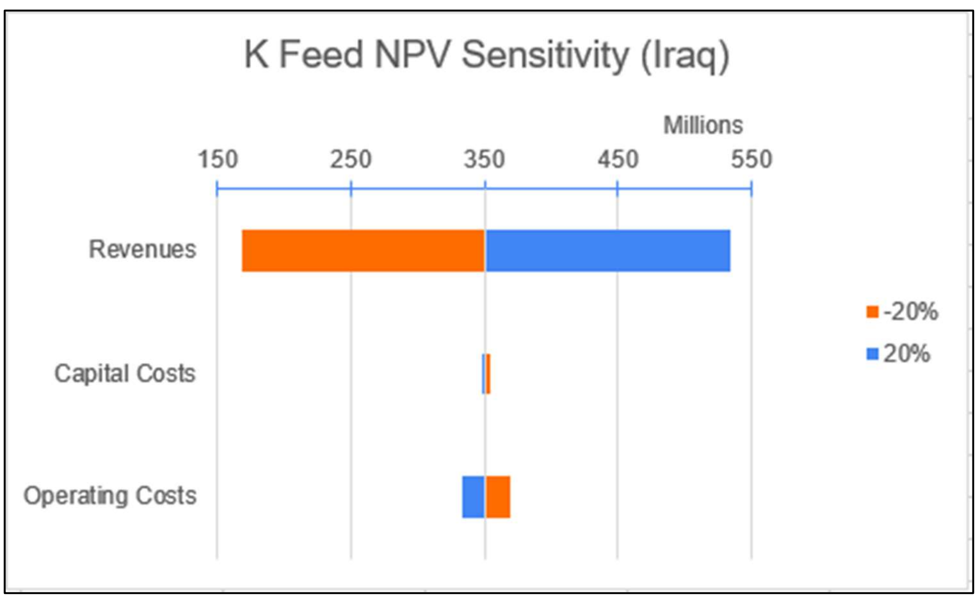

Figure 6: K Feed NPV Sensitivity (Iraq)

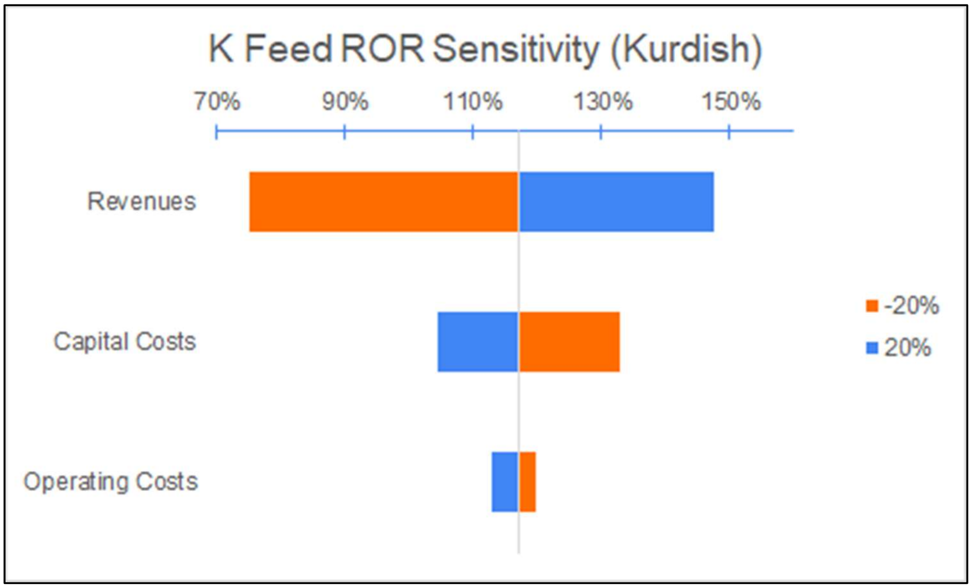

Figure 7: K Feed ROR Sensitivity (Kurdish)

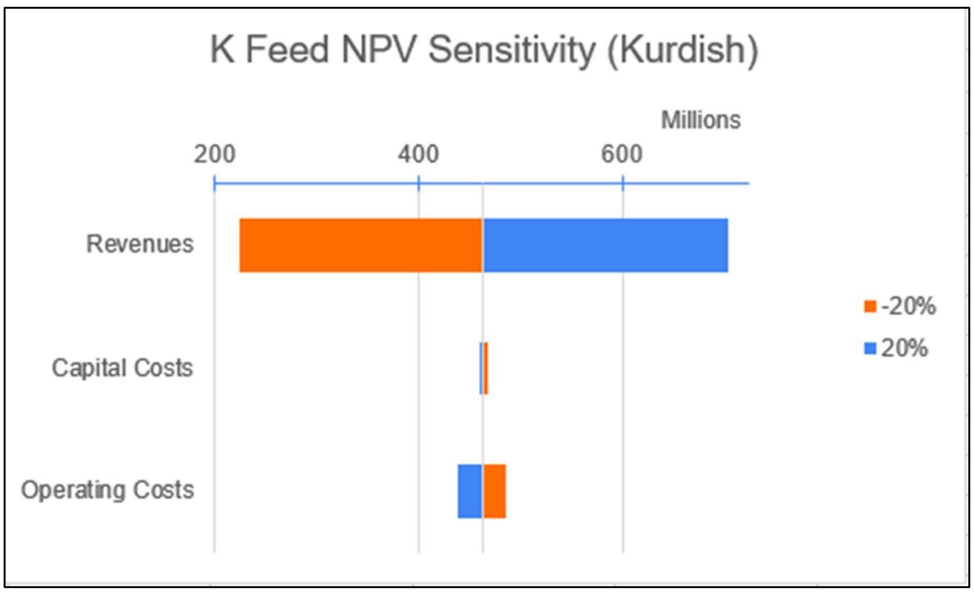

Figure 8: K Feed NPV Sensitivity (Kurdish)

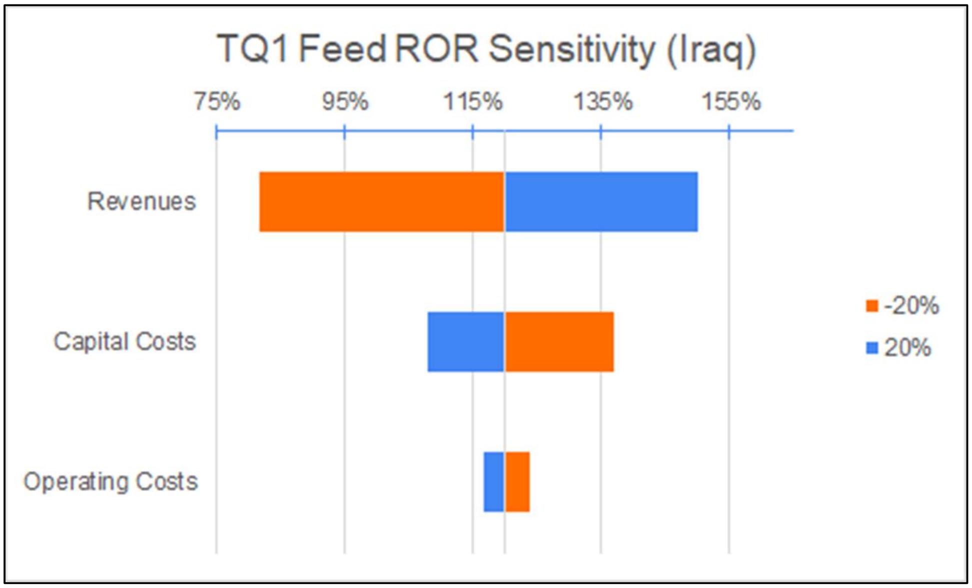

Figure 9: TQ1 Feed ROR Sensitivity (Iraq)

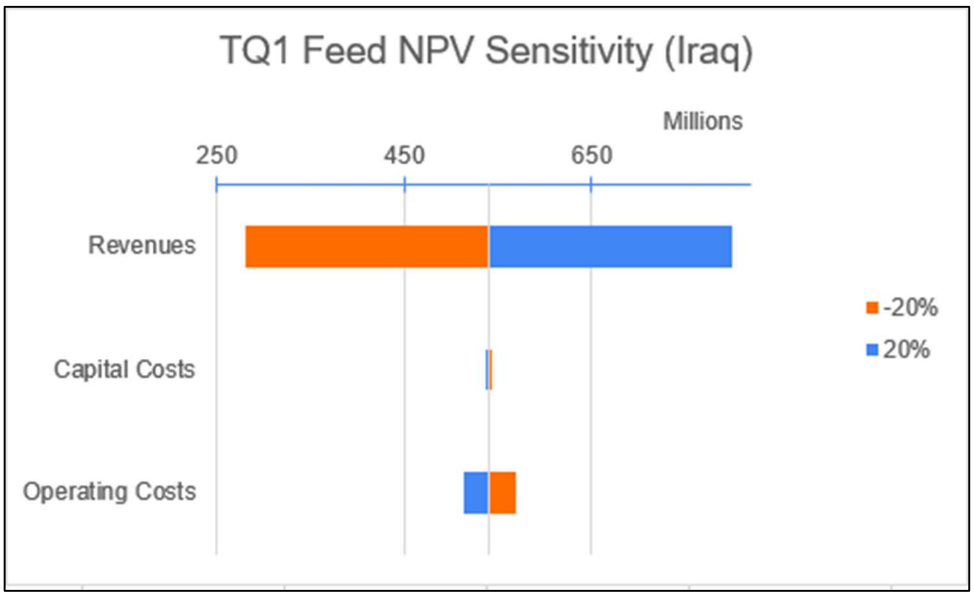

Figure 10: TQ1 Feed NPV Sensitivity (Iraq)

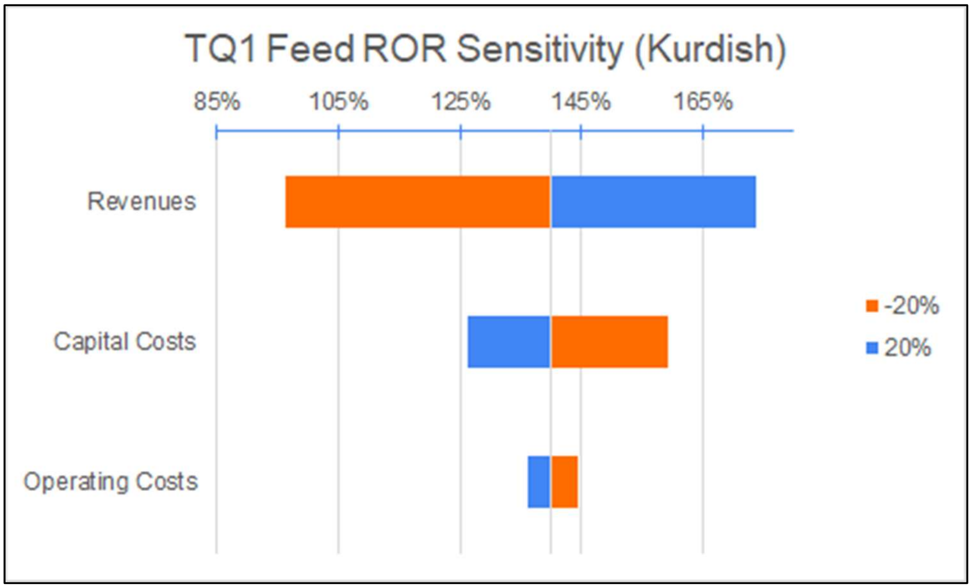

Figure 11: TQI Feed ROR Sensitivity (Kurdish)

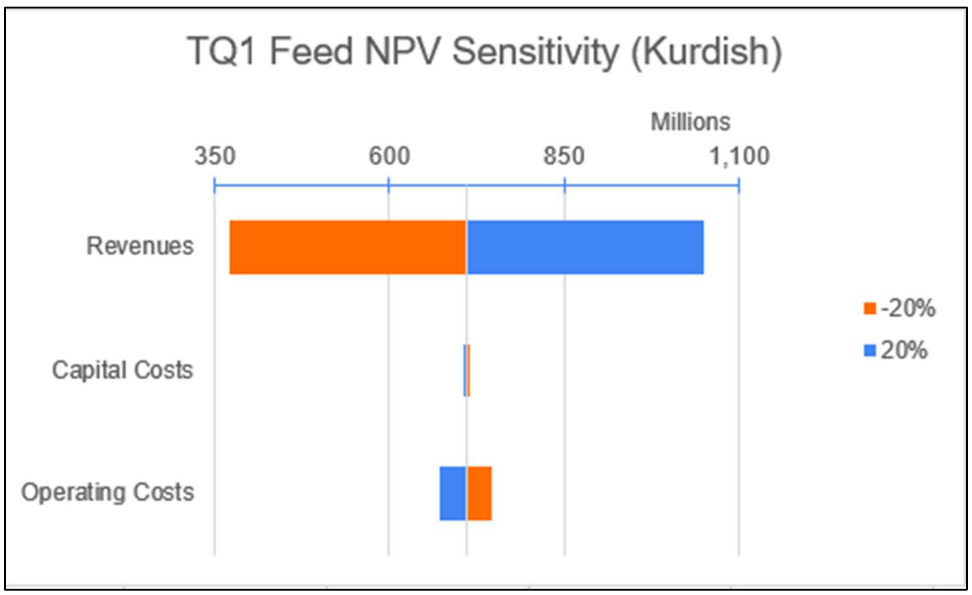

Figure 12: TQ1 Feed NPV Sensitivity (Kurdish)

From the results, product revenue has the most major effect on the NPV and ROR. On the other hand, the fixed capital cost and annual operating costs did have an impact, but with minimal results in comparison. Going forward, the most important aspect to maximize would be the profitability for the project in product production. Ensuring that production is maximized, the higher operating or fixed capital cost associated with a higher production rate would be outweighed by the heightened income.

Process Safety

Inherent Safety Evaluation

The process that is used to accommodate the goal of converting the naphtha feedstock from Mr. Abbasi's refinery utilizes several aspects of inherently safer design in order to both reduce hazards and eliminate risk in the process. The first aspect is moderation. This is most evident in the extraction and distillation sections as the group elected to use lower operating pressures for the columns in these sections. By running the process at lower pressures, there is a significant reduction in the risk that a vessel rupture will occur and reduces the threat of large-scale damage in the event of a vessel rupture. The lower pressures also allow for lower operating temperatures which, in turn, allow for chemicals in these sections to be processed at conditions that would make them less hazardous should an incident occur. The second aspect is simplification. By reducing the number of excess units in the process, the group was able to reduce the number of potential sources of risk in the overall process. The only units added from the original rough draft PFD are two additional pumps in the extraction section and distillation section respectively. The inherent complexity of other units is also kept to a minimum with the only exception being the addition of specially picketed weir trays for Stripper 2[2]. The third aspect is minimization. The group reduced the inflow of Sulfolane in the extraction section which creates an overall safer process as flow rates through columns in this section are reduced leading to better overall safety. This also reduced the need to store large amounts of Sulfolane in feed tanks on site. In addition to this, the group added cooling jackets to each packed-bed reactor in the reaction section. While the temperatures in reactors 1 and 2 decrease and the temperature in reactor 3 only increases slightly, the group felt that this was an important addition to the section as the threat of a runaway reaction in the reverse direction could be catastrophic, especially at the high temperatures and pressures the reactors operate at. By flowing cooling water, the group can minimize the reactor temperature if needed and prevent runaway reactions. The final aspect is substitution. The group chose to utilize the 150-psig steam utility in all but two columns in the K feed process. In all other columns, the amount of steam needed was higher overall but by using the less hazardous 150-psig steam, the group was able to operate at safer pressures and temperatures and increase process safety overall. In the two columns, the temperature requirement could not be attained without use of the 450-psig steam. These four aspects play a critical role in the safe and effective operation of this chemical plant but reducing the overall risk of the process and increasing the inherent safety of the process writ large.

Process Safety Management

Process hazards

Throughout this process, there are several component hazards that should be accounted for in both the design of the overall plant and in plant operation. The group examined the health, flammability, and toxicity concerns for all chemicals used in this process by using data from OSHA, NFPA, and the Hazardous Substances Data Bank[3,4,5]. All relevant data is shown below in Table 10 however, the group would like to highlight several key areas.

Component	OSHA Chemical Exposure Limit	NPFA Safety Diamond Classifications				Lethal Dose (LD_{50}) limits
		Health	Fire	Reactivity	Special	
n-decane	N/A	1	2	0	None	N/A
cyclohexane	300 ppm	1	3	0	None	8.0 - 39.0 mL/kg
benzene	10 ppm	1	3	0	None	3306 mg/kg
hydrogen	N/A	0	4	0	None	N/A
methane	Simple Asphyxiant (at least 18% O2)	2	4	0	None	15400 mg/kg
ethane	N/A	1	4	0	None	N/A
propane	1000 ppm	2	4	0	None	N/A
n-butane	800 ppm (enforced in some states)	1	4	0	None	N/A
n-pentane	1000 ppm	1	4	0	None	446 mg/kg (mouse intravenous)
n-hexane	500 ppm	0	3	0	None	45 mL/kg
n-heptane	500 ppm	1	3	0	None	75 g/(m3*hr) (mouse inhalation)
n-octane	500 ppm	1	3	0	None	N/A
n-nonane	200 ppm (NIOSH 10 hour TWA)	1	3	0	None	218 mg/kg (mouse iv)
toluene	200 ppm	2	3	0	None	2.6 - 7.5 g/kg
p-xylene	100 ppm	2	3	0	None	5 g/kg
Sulfolane	N/A	2	1	0	None	1941 mg/kg
water	N/A	N/A	N/A	N/A	N/A	25000 mg/kg (mice)
air	N/A	N/A	N/A	N/A	N/A	N/A
oxygen	N/A	3	0	0	Oxidizer	N/A
nitrogen	Simple Asphyxiant (at least 18% O2)	3	0	0	None	N/A
carbon monoxide	50 ppm	3	4	0	None	4000 ppm in one hour (humans)
carbon dioxide	5000 ppm	3	0	0	None	N/A
	Unless stated, all are based on 8 hour TWA	*Pubchem data from the Hazardous Substances Data Bank*				
	Unless stated,OSHA PEL Z-1 and Z-2 tables				*LD_{50} limits in rats unless stated otherwise*	

Table 12: OSHA, NPFA, and LD50 Data

First is benzene which is one of the desired products from this process. benzene has the lowest OSHA chemical exposure limit of 10 ppm and has an LD_{50} limit of 3306 mg/kg. This means that the handling of Benzene should be treated with serious caution throughout the process. The second key hazardous component is carbon monoxide which has an OSHA chemical exposure limit of 50 ppm and an LD_{50} limit of 4000 ppm in one hour. While no stream in our process has a composition that includes the presence of carbon monoxide, it can still form as a product of incomplete combustion and its potential presence in the fired heater flue gas should be considered due to its hazardous properties. The final key area is regarding the numerous hydrocarbons present in the process. All these hydrocarbons have an NFPA flammability rating of at least 2 with most being rated 3 to 4. These high ratings mean that special precautions should be taken in the arena of fire protection as even the smallest leak of these chemicals could pose a serious safety issue. No component in this process has a reactivity rating of greater than 0 and no component, other than oxygen, has a special rating from the NFPA. Thus, no additional personal protective equipment (PPE) needs to be utilized for these hazards. Operators should maintain the uses of protective eyewear, hardhats, and other basic PPE when onsite. Material safety data sheets should also be accessible at each apparatus, so operators are aware of the chemicals present in each area of the plant.

P&ID of the Major Fractionator

In order to further promote safe operation, the group created a basic P&ID for the process "major fractionator" utilizing best available control technology (BACT). The P&ID shows several control loops that govern the first distillation column (Distillation Column T-106) in the PFD). The control loops are broken down into loops that govern the tower and loops that govern the condenser, reflux drum, and reboiler. The tower is regulated by a level control loop at the bottom and a pressure control loop at the top. The condenser has two temperature control loops which can adjust the cooling water inlet to account for temperature changes in the flow to the condenser and the cooling water outlet. The reflux drum has a level control loop to prevent overflow. The reboiler has a temperature control loop which can adjust the flow of saturated steam to account for changes in the temperature of the flow to the reboiler. All pressure and level control loops are equipped with high- and low-level alarms to alert operators should dangerous conditions arise in regard to these areas. Finally, a pressure relief valve has been installed on the column in the event that the column becomes over pressured to a point that the first pressure control loop cannot fix. This valve must have an area of at least 16.1 square inches[6] and the group has determined that the use of a Crosby J-Series Direct Spring Pressure Relief Valve can be used to accommodate this[7]. The full P&ID of the major fractionator (Distillation Column T-106) is shown below in Figure 13.

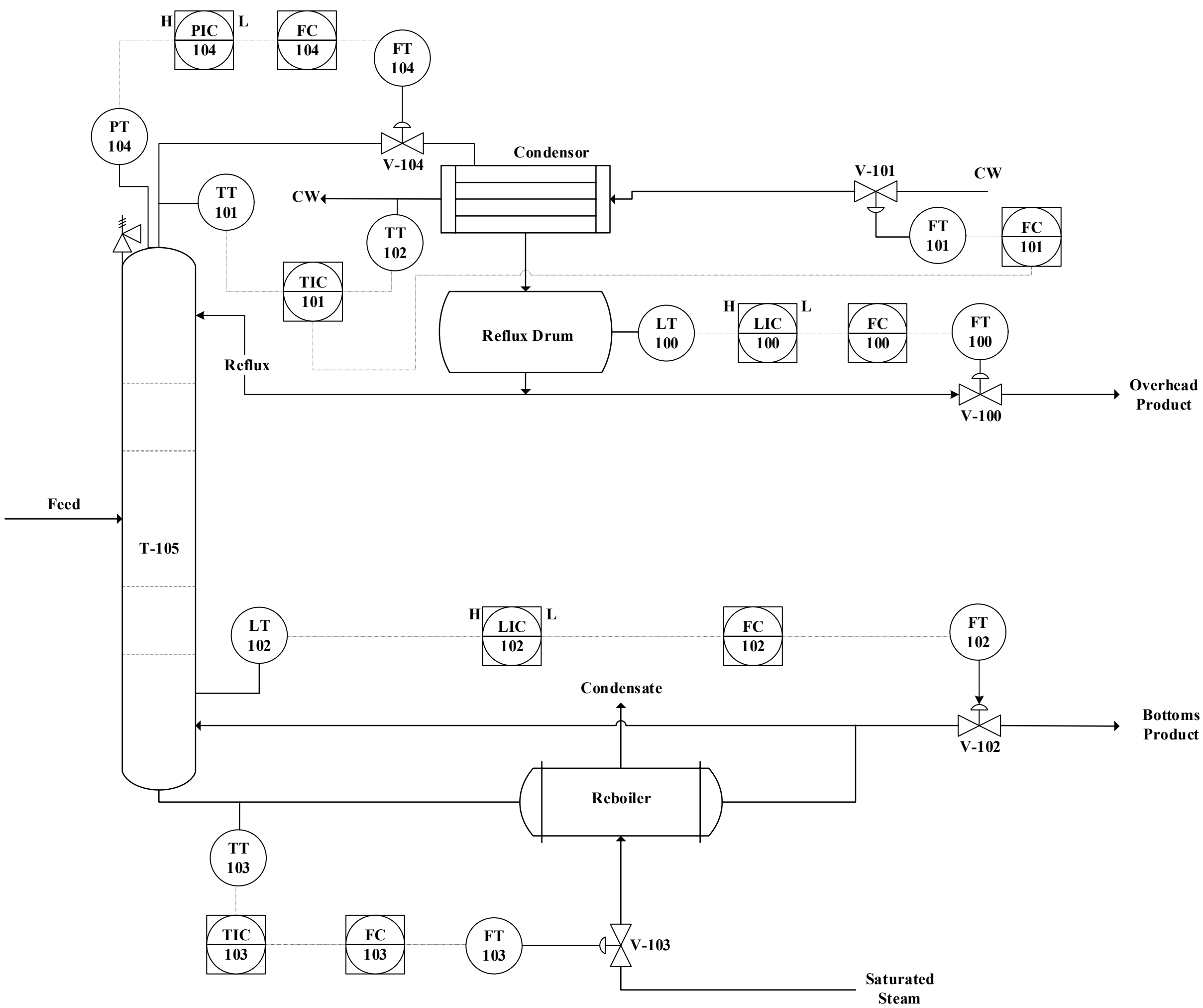

Figure 13: P&ID of Major Fractionator

Uncongested Vapor Cloud Deflagration

Hydrocarbon explosions pose perhaps the greatest potential for large scale disaster. In order to account for this possibility, the group evaluated the worst-case scenario for a hydrocarbon release and explosion from the major fractionator (Distillation Column T-106) in the K feed simulation. The group assumed that all materials in the column had a heat of combustion equivalent to n-decane, which had the largest heat of combustion of all materials, an empirical explosion efficiency of 0.1, and an ambient pressure of 101.325 kPA. The group also assumed that the explosion took place on the ground since this would result in the maximum possible destruction. A TNT-equivalency calculation determined that this explosion would be equal to 14.93 kg to TNT[8]. Further analysis shown in Table 11[8] shows the destruction that would occur at various distances from the blast location.

Distance from Ground Zero (m)	Scaled Distance (m/kg^1/3)	Scaled Overpressure	Peak Side-On Overpressure (kPa)	Damage Estimates for Common Structures
10	4.061	0.8	81.06	Total Destruction
50	20.3056	0.084	8.511	Corrugated asbestos shatters; corrugated steel or aluminum panels fastenings fail, followed by buckling; wood panels fastenings fail, panels blow in. Partial demolition of houses, made uninhabitable
100	40.611	0.04	4.053	Large and small windows shatter; occassional damage to window frames. Limited minor structural damage
250	101.528	~0.01	1.013	Near typical pressure of glass breakage. Small windows shatter if under strain
500	203.056	~0.005	0.507	Loud noise and occasional breakage of large glass windows if under strain
Based on calculations, a distance of approximately 150m is considered "safe" in accordance with Table 6-9				

Table 13: Damage at Distance from Blast

Based on this information, the group has determined that distance of approximately 150m from the blast site is considered “safe”. Finally, the group examined the upper and lower explosive limits of all components present in the column and the results are shown in Table 12[5].

Explosive Limits (Components in T-106)		
Component	Lower Explosive Limit (LEL)	Upper Explosive Limit (UEL)
n-decane	0.80%	2.60%
benzene	1.2 % (OSHA)	8% (OSHA)
p-xylene	1.10%	7%
toluene	1.1% (OSHA)	7.1% (OSHA)
heptane	1.05% (OSHA)	6.7% (OSHA)
octane	1.0% (OSHA)	6.5% (OSHA)
nonane	0.8% (OSHA)	2.9% (OSHA)
sulfolane	N/A	N/A
All data from CAMEO Chemicals database unless otherwise listed		

Table 14: Upper and Lower Explosive Limits

This scenario represents a worst case because in reality, the heat of combustion for the components in the column are all less than, and in some cases significantly less than, n-decane.

However, should the flow of hydrocarbons to the column be increased substantially, a new TNT-equivalency calculation should be performed to evaluate for potential destruction.

Safety Summary

Overall, the hazards associated with this process do not radically differ from the common process hazards found in today's modern hydrocarbon industry. The components that the process utilizes do not possess abnormal toxicity or reactivity, however they are extremely flammable and do pose health risks to operators if proper precautions are not taken. The major fractionator (Distillation Column T-106) can be regulated by several control loops and a relief device in order to ensure safe operation and modelling for the worst-case scenario of a hydrocarbon explosion shows how the plant should be orientated with respect to control rooms and areas where personnel are present. The plant's great strength rests in its inherently safer design which applies minimization, substitution, moderation, and simplification to reduce risks across the entire plant. The group does recommend that special attention be paid to the reaction section as the reactors and fired heater operate and the highest temperatures and pressures in the plant. Future analysis would involve the sizing of individual pressure relief devices, such as rupture disks, for each packed-bed reactor and a plant-wide P&ID would be drafted to implement control loops and relevant alarms and sensors in all apparatuses. In addition to this, a specific quote for the Crosby J-Series Direct Spring Pressure Relief Valve[7] should be acquired to produce more accurate costing in regard to safety.

Conclusions

After completing the preliminary economic analysis for both the TQ1 and K naphtha feeds of the proposed refinery design, the group has determined that this project is economically attractive. For feed K, this project has an NPV of $467,034,757 in Kurdish and an NPV of $353,689,661 in Iraq. Feed TQ1 has an NPV of $714,142,721 in Kurdish and an NPV of $542,288,196 in Iraq. Feed K has a DCROR of 99% and 117% in Iraq and Kurdish respectively, while the DCROR values for TQ1 are 121% and 140% in Iraq and Kurdish, respectively. Based on these numbers, both feeds could be implemented into Mr. Abbasi's refinery profitably, although based on the net present value and discounted cash flow rate of return, feed TQ1 proves to be considerably more profitable. In conclusion, the group recommends Mr. Abbasi's refinery implements this design for either feed K or TQ1. Although both feeds are profitable, and feed K is of greatest interest, stream TQ1 proves to be the most profitable.

In addition to this, both feeds are able to be processed under relatively safe conditions without the need for specialized equipment to handle specific chemicals or operations. Both designs implement inherently safer design steps to reduce risks and minimize hazards for operators. Key apparatuses analyzed in both feeds can utilize control loops and pressure relief devices to prevent disaster and uphold process integrity. Along with this, the worst-case scenarios examined in both designs in terms of a hydrocarbon explosion can be prepared for by implementing a plant layout that protects operators and further minimizes risk.

There are still several possible areas in which the process could be further improved. The first involves the recycle ratio of hydrogen to the reactor section. It may be possible to further increase conversion by modifying the recycle ratio to an optimum level. However, further analysis is needed to determine the viability of adjusting this ratio. Another area involves the elimination of benzene loss out of the first stripper (T-100). The overhead outlet of this stripper is causing valuable benzene to be lost instead of being sent further into the extraction section. By eliminating this loss, the amount of benzene product being generated would increase and result in higher yearly revenues. The final area involves the high temperatures in the reboilers for several strippers. The 450-psig steam provided is the most expensive heating utility available and, as a result, leads to a higher operating cost for the process in both the K feed and the TQ1 feed. If there was a way to reduce the operating temperature in these reboilers such that the 150-psig steam could be utilized, then the process operating costs would be reduced and the reboilers would be safer to operate.

Appendix

a. Reactor Train Detail

The reactor section design utilizes three packed-bed reactors with a fired heater used to reheat the process streams entering each reactor. The reactors are each based on the reaction kinetics provided in the 1959 Naphtha Reforming article[9] and are described in rate law form in Figure 14 where rate is in kmol/m3, pressure is in MPa, and temperature is in K.

$$rate = 9.4928 * 10^{13} e^{\frac{-160506.4}{8.314T}} P_{C_6H_{12}} - 8.2728 * 10^{-4} e^{\frac{52170.4}{8.314T}} P_{C_6H_6} P_{H_2}^3$$

$$rate = 3.6704 * 10^{21} e^{\frac{-287756.8}{8.314T}} P_{C_6H_{12}}$$

$$rate = 3.6704 * 10^{21} e^{\frac{-287756.8}{8.314T}} P_{C_{10}H_{22}}$$

$$rate = 3.33674 * 10^{19} e^{\frac{-275285.8}{8.314T}} P_{C_6H_{12}} P_{H_2} - 4.19816 * 10^{21} e^{\frac{-312237.9}{8.314T}} P_{C_6H_{12}}$$

Figure 14: Rate Law Data

The choice of operating temperatures and pressures were also determined from this article as the rate law data was found at the temperature of 943 °F and 586 psia. Thus, the fired heater was designed to heat or reheat streams using natural gas and air to a temperature of 943 °F in order to maintain consistency. The reactors each used a catalyst for the hydrocracking of the feed stream to generate lighter hydrocarbons and desirable benzene. The cracking process is the key component of the reactor section and, upon further research, the group selected to use the BASF NaphthaMax[10] catalyst in each reactor. The catalyst was assumed to have an average catalyst lifespan of five years and modeled with a void fraction of 0.8 in each reactor[11]. Exact cost of the catalyst is not known however the catalyst is an aluminum oxide catalyst with a low weight percentage of sodium oxide. To estimate price, the group found a comparable catalyst that was composed of these same chemicals with sodium oxide in a relatively similar weight percentage[12]. The product leaving the reaction section enters a vapor feed separator which sends the liquids to the extraction section and the vapors to either be used elsewhere as light hydrocarbons or recycled back into the stream entering the fired heater. By using a recycle ratio of 0.5, the group was able to combine the recycle stream with the inlet naphtha stream and reduce the pressure in the reactors to no more than 224 psia. This increased the safety of the process and maintained a strong conversion rate. The group also elected to use a cooling jacket on each reactor to prevent runaway reactions. While there is normally a temperature drop across the reactors, reactions in the reverse direction are exothermic and a change in the composition of the feed stream could cause safety concerns. In order to appropriately cost utilities for this jacket, the group assumed that the jacket would be turned on for eight weeks over the course of a nine-year period. The bare module costs and yearly operating costs for the reaction section are shown in Table 13.

Reaction Section Costs Overview (K feed)	
Cost Category	**Cost Value**
Total Bare Module Cost	$ 8,079,480
Total Operating/Labor Costs	$ 293,480
Total Utility Costs	$ 4,458,021

Table 15: Reaction Section Costs Overview (K feed)

b. Exactor Section Detail

The extraction section consists of a pump, three coolers, two liquid-liquid extractors, three stripping columns with reboilers and reboiler pumps, and a distillation column with a condenser, reboiler, and their corresponding pumps. The key aspect of this section involves the specification of certain binary interaction parameters. The group used scholarly research regarding systems containing the important components to determine these parameters[13]. The overall design of this section was also based on research of systems involving sulfolane-based extraction[14]. The first and third stripping columns have valve trays, and all other columns were designed with sieve trays with special picketed weirs being used in the second stripping column[2]. This section extracts the other stream components to form a reformate stream consisting of benzene, toluene, and xylene known as the BTX stream. The process stream coming in from reaction section is first cooled to 212°F before entering the first stripping column (T-100) at 8.1 bar. This column removes the lighter hydrocarbons to create a stream of n-decane and benzene. The reboiler operates at 441°F and 8.5 bar. The temperature profile is shown in Figure 15.

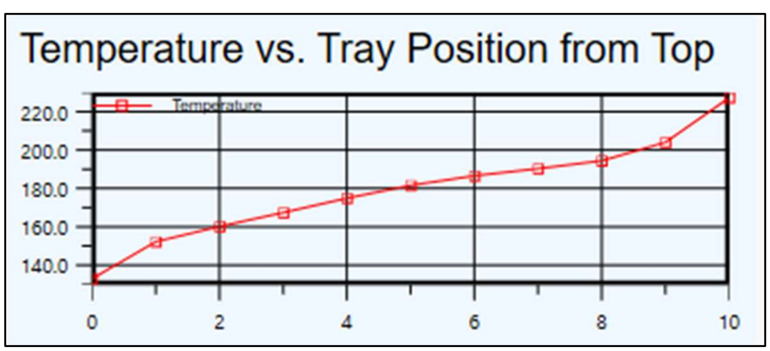

Figure 15: Temperature Profile in T-100

The bottoms product from the stripper is then mixed with a recycle stream coming from the bottom product of Distillation 1 (T-106) before flowing into a cooler. The cooler reduces the temperature to 95°F and a pressure of 1.4 bar before flowing into the bottom of the first liquid-liquid extractor (T-102). The top stream coming into T-102 consists of a mixture of a recycle stream from the bottom of stripping column 2 (T-104) a recycle stream from the bottom of stripping column 3 (T-105) and sulfolane. This mixed stream is cooled to 95°F with E-104 and the pressure raised to 1.6 bar by Pump 101 before entering the extractor. The extractor temperature profile is illustrated in Figure 16.

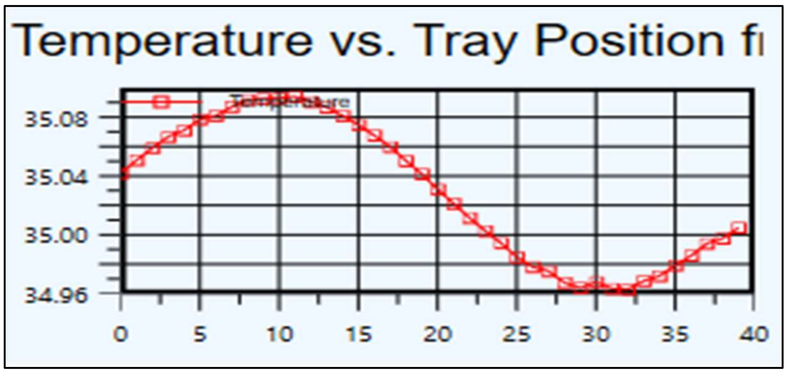

Figure 16: Temperature Profile in T-102

The top product of T-102 flows into the second liquid-liquid extractor (T-103) along with a water inlet stream. This extractor operates at 1.6 bars with the temperature profile presented in Figure 17.

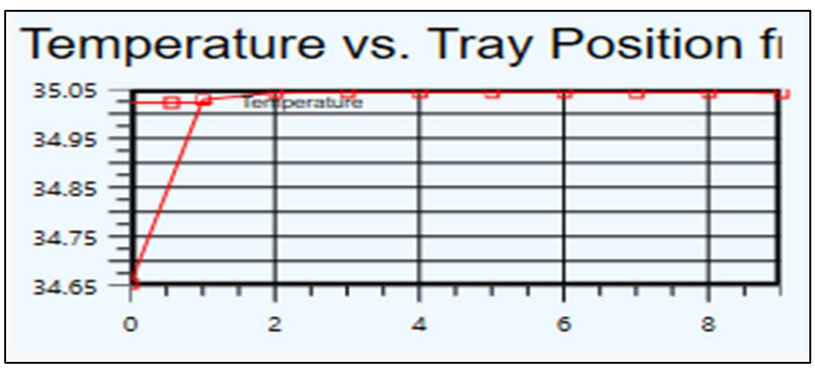

Figure 17: Temperature Profile in T-103

The product stream continues from T-103 to the second stripping column (T-104). This column operates at 1.8 bar with its temperature profile displayed in Figure 18.

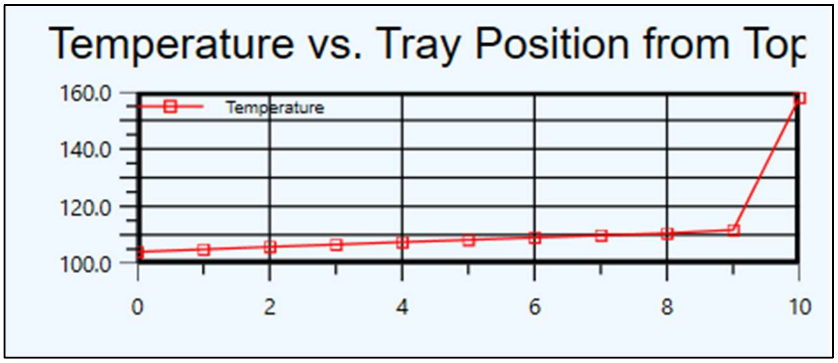

Figure 18: Temperature Profile in T-104

The bottom product from the first extractor (T-102) flows into the third stripping column (T-105). This column is operated at 1.8 bar with the temperature profile shown in Figure 19.

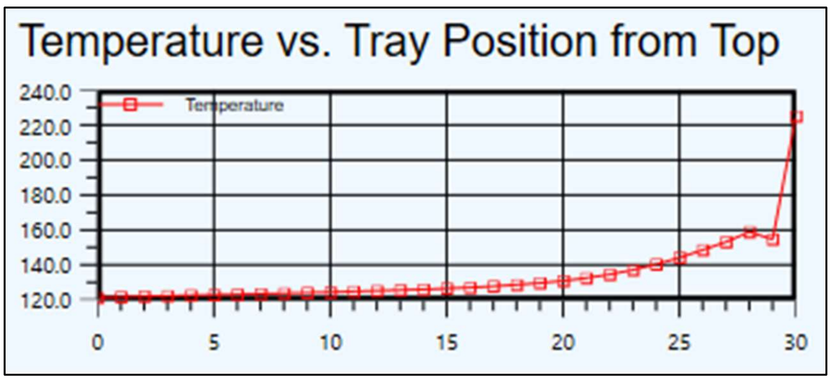

Figure 19: Temperature Profile in T-105

The product stream from T-105 flows into distillation 1 (T-106). The top product from T-106 continues to the distillation section. This column operates at 1.6 bar with the temperature profile illustrated below in Figure 20.

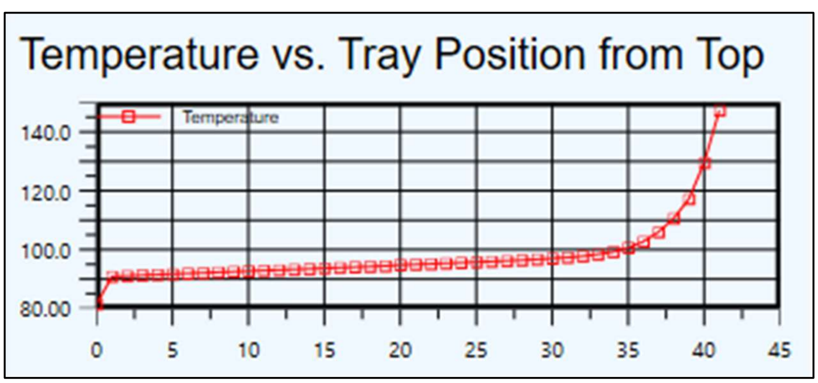

Figure 20: Temperature Profile in T-106

Sizing and heuristics for apparatuses in this section utilize various sources[15,16,17,18]. The bare module capital cost and yearly operating cost outlined for this section is shown in Table 14.

Extraction Section Costs Overview (K feed)	
Cost Category	**Cost Value**
Total Bare Module Cost	$ 3,688,685
Total Operating/Labor Costs	$ 617,904
Total Utility Costs	$ 2,416,342

Table 16: Extraction Section Costs Overview (K feed)

This design is currently operated recycling 99% of the sulfolane feed with a cost of $4,490,000 per year. If the sulfolane was reduced to only recycling 90% the cost increased to $427,700,000 per year.

c. Distillation Section Detail

The distillation section is the last section in the design process, and utilizes one pump, one cooler, and two distillation columns along with their respective condensers, reboilers and pumps. The purpose of this section is to completely separate the BTX reformate mixture into its original components of benzene, toluene, and xylene. After leaving the extraction section, the feed K BTX stream is pumped to a pressure of 2 bar, and then cooled to 140°F before entering the first distillation column (T-107). The purpose of this column is to separate benzene from the toluene and xylene mixture as purely as possible. The group chose to run this column with a reflux ratio of 4, and with a pressure of 1.4 bar in the condenser and 1.765 bar in the reboiler. The number of stages for this column was found to be 25, after finding the minimum stage number and dividing by the column's efficiency. The temperature of the column ranges from 175°F in the condenser to 286°F in the reboiler. Based on these temperatures calculated by Aspen HYSYS, 150 psig steam was used in the reboiler and cooling water at 77°F was used in the condenser. A temperature profile for T-107 is shown below in Figure 21. Because benzene is more volatile than both toluene and xylene, the distillation column at these parameters was able to separate benzene into the distillate outlet at 75% purity while the toluene and xylene flows through the bottoms of the first column into the second column.

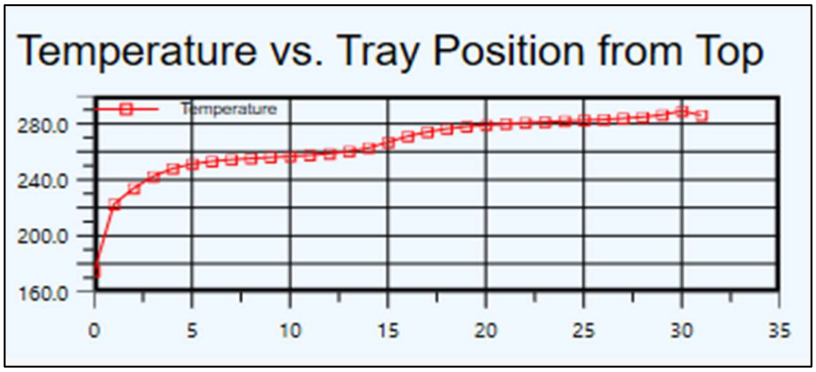

Figure 21: Temperature gradient of Distillation 2 (T-107)

The second and final column in the distillation section (T-108) separates toluene and para-xylene. Based on the relative volatilities of these two compounds, toluene is separated in the distillate product and para-xylene is separated in the bottom product. This column has a pressure of 1.5 bar in the condenser and 3 bar in the reboiler, with a reflux ratio of 1.87 and an actual stage number of 22 stages, based on minimum stage number and column efficiency. The temperatures in the column range from 257°F in the condenser to 367°F in the reboiler. Similar to T-107, the reboiler uses 450 psig steam and the condenser uses the cooling water supplied to the refinery. A temperature profile for this column is shown below in Figure 22.

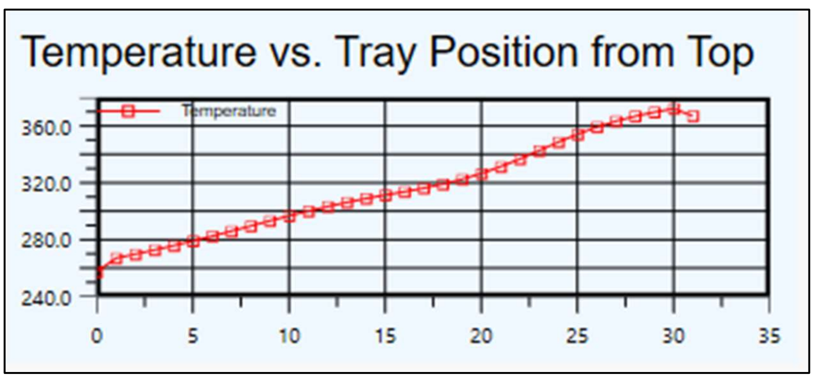

Figure 22: Temperature Gradient of Distillation 3 (T-108)

An issue arose during simulation that the group had to fix involving a small percentage of water in the BTX stream entering the distillation towers, which was causing a problem of two phases present in the condenser. When this issue arose, the group lowered the temperatures coming out of the coolers in the extraction section as well as cooler E-108 before the stream entered the first column in the distillation section, which successfully fixed the problem and removed the water from the column. Both columns were designed and priced using sieve trays. Trays were chosen for the columns instead of packing based on a lower price when both options were analyzed, and sieve trays were chosen based on the column optimization within Aspen

HYSYS internals to prevent any flooding or weeping in the trays. The material of construction choice for both columns was carbon steel because no corrosive substances are being processed through the columns. Sizing and heuristics for apparatuses in this section utilize various sources[15,16,17,18]. The bare module capital cost of all equipment in the distillation section is shown below in table 15.

Distillation Section Costs Overview (K feed)	
Cost Category	**Cost Value**
Total Bare Module Cost	$ 1,277,686
Total Operating/Labor Costs	$ 308,952
Total Utility Costs	$ 851,107

Table 17: Distillation Section Costs Overview (K feed)

Equipment Summary Table for Feed K						
Section	**Description**	**PFD Label**	**Design Temperature (F)**	**Design Pressure (Bar)**	**Design Parameter**	**Size**
Heater/Furnace	Fired Heater (K Feed)	H-100	928	14.7	Heater Duty (kW)	22,961.0
Reactors	Reactor I	R-100	943	16.3	Volume (m^3)	284.7
	Reactor II	R-102	943	17.9	Volume (m^3)	294.5
	Reactor III	R-103	949	17.2	Volume (m^3)	294.5
Process Vessel	Stripper I	T-100	441	13.4	Volume (m^3)	20.7
	Stripper II	T-105	316	6.4	Volume (m^3)	6.4
	Stripper III	T-104	437	81.7	Volume (m^3)	4.3
	Column I	T-106	297	4.1	Volume (m^3)	19.2
	Column II	T-107	286	4.3	Volume (m^3)	10.0
	Column III	T-108	367	4.2	Volume (m^3)	47.5
	Liquid Extractor I	T-102	95	4.3	Volume (m^3)	32.6
	Liquid Extractor II	T-103	94	4.3	Volume (m^3)	43.5
Condensers	Column I Condenser	E-107	179	3.6	Condenser Duty (Btu/hr)	6,268,720.0

	Column II Condenser	E-109	175	3.8	Condenser Duty (Btu/hr)	1,392,770.0
	Column III Condenser	E-111	257	3.8	Condenser Duty (Btu/hr)	11,426,800.0
Reboilers	Stripper I Reboiler	E-102	441	10.8	Condenser Duty (Btu/hr)	7,818,000.0
	Stripper II Reboiler	E-106	316	3.6	Condenser Duty (Btu/hr)	973,200.0
	Stripper III Reboiler	E-105	437	4.1	Condenser Duty (Btu/hr)	18,400,000.0
	Column I Reboiler	E-108	297	3.9	Condenser Duty (Btu/hr)	5,093,000.0
	Column II Reboiler	E-110	286	4.1	Condenser Duty (Btu/hr)	1,848,000.0
	Column III Reboiler	E-112	367	4.1	Condenser Duty (Btu/hr)	11,420,000.0
Pumps	Naphtha A/B	P-100	164	43.9	Purchased hp (kW)	71.7
	P-101 A/B	P-101	95	4.0	Purchased hp (kW)	0.8
	BTX A/B	P-102	179	4.2	Purchased hp (kW)	0.1
	Stripper I Reboiler A/B	N/A	425	160.0	Purchased hp (kW)	2.6
	Stripper II Reboiler A/B	N/A	316	21.0	Purchased hp (kW)	0.0
	Stripper III Reboiler A/B	N/A	437	28.0	Purchased hp (kW)	5.3
	Column I Reboiler A/B	N/A	297	22.0	Purchased hp (kW)	0.0
	Column II Reboiler A/B	N/A	286	25.0	Purchased hp (kW)	0.4
	Column III Reboiler A/B	N/A	367	45.0	Purchased hp (kW)	0.2
	Column I Condenser A/B	N/A	178	18.0	Purchased hp (kW)	0.5
	Column II Condenser A/B	N/A	175	20.0	Purchased hp (kW)	0.1
	Column III Condenser A/B	N/A	258	21.0	Purchased hp (kW)	0.4
Reflux Drums	Column I Condenser Drum	N/A	179	3.6	Volume (m^3)	6,268,720.0

	Column II Condenser Drum	N/A	175	3.8	Volume (m^3)	1,392,770.0
	Column III Condenser Drum	N/A	257	3.8	Volume (m^3)	11,426,800.0
Heat Exchangers	Cooler I	E-100	347	14.0	Cooler Duty (Btu/hr)	51,283,449.5
	Cooler II	E-101	117	10.9	Cooler Duty (Btu/hr)	4,173,156.1
	Cooler III	E-102	95	9.2	Cooler Duty (Btu/hr)	4,173,156.1
	Cooler IV	E-103	95	9.2	Cooler Duty (Btu/hr)	16,061,575.2
	Cooler V	E-104	140	9.2	Cooler Duty (Btu/hr)	96,975.8
Separators	Vapor Feed Separator	V-101	347	8.8	Volume (m^3)	3.7

Table 18: Equipment Summary Table for Feed K

Equipment Summary Table for Feed TQ1						
Section	**Description**	**PFD Label**	**Design Temperature (F)**	**Design Pressure (Bar)**	**Design Parameter**	**Size**
Heater/Furnace	Fired Heater (K Feed)	H-100	943	22.6	Heater Duty (kW)	26,041.0
Reactors	Reactor I	R-100	943	22.6	Volume (m^3)	284.7
	Reactor II	R-102	938	23.3	Volume (m^3)	294.5
	Reactor II	R-103	943	23.3	Volume (m^3)	294.5
Process Vessel	Stripper I	T-100	426	8.5	Volume (m^3)	20.7
	Stripper II	T-105	363	1.3	Volume (m^3)	6.4
	Stripper III	T-104	437	1.8	Volume (m^3)	81.7
	Column I	T-106	255	1.6	Volume (m^3)	19.2
	Column II	T-107	285	1.8	Volume (m^3)	10.0
	Column III	T-108	367	3.1	Volume (m^3)	10.0
	Liquid Extractor I	T-102	95	1.6	Volume (m^3)	26.4
	Liquid Extractor II	T-103	95	1.6	Volume (m^3)	43.5

Condensers	Column I Condenser	E-107	180	1.2	Condenser Duty (Btu/hr)	7,692,460.7
	Column II Condenser	E-109	170	1.4	Condenser Duty (Btu/hr)	1,010,323.0
	Column III Condenser	E-111	257	1.5	Condenser Duty (Btu/hr)	22,675,072.2
Reboilers	Stripper I Reboiler	E-102	437	8.5	Condenser Duty (Btu/hr)	10,539,001.3
	Stripper II Reboiler	E-106	363	1.3	Condenser Duty (Btu/hr)	803,075.1
	Stripper III Reboiler	E-105	437	1.8	Condenser Duty (Btu/hr)	35,850,803.3
	Column I Reboiler	E-108	255	1.6	Condenser Duty (Btu/hr)	6,128,000.0
	Column II Reboiler	E-110	285	1.8	Condenser Duty (Btu/hr)	1,533,079.6
	Column III Reboiler	E-112	367	3.1	Condenser Duty (Btu/hr)	22,753,760.7
Pumps	Naphtha A/B	P-100	164	42.7	Purchased hp (kW)	94.3
	P-101 A/B	P-101	95	4.0	Purchased hp (kW)	1.7
	BTX A/B	P-102	179	4.2	Purchased hp (kW)	0.1
	Stripper I Reboiler A/B	N/A	426	122.9	Purchased hp (kW)	4.1
	Stripper II Reboiler A/B	N/A	363	18.3	Purchased hp (kW)	0.0
	Stripper III Reboiler A/B	N/A	437	25.6	Purchased hp (kW)	12.3
	Column I Reboiler A/B	N/A	297	22.8	Purchased hp (kW)	0.1
	Column II Reboiler A/B	N/A	286	25.6	Purchased hp (kW)	0.5
	Column III Reboiler A/B	N/A	367	45.0	Purchased hp (kW)	0.1
	Column I Condenser A/B	N/A	178	18.1	Purchased hp (kW)	0.5
	Column II Condenser A/B	N/A	175	20.4	Purchased hp (kW)	0.1
	Column III Condenser A/B	N/A	258	21.8	Purchased hp (kW)	0.3

Reflux Drums	Column I Condenser Drum	N/A	180	1.2	Volume (m^3)	5.7
	Column II Condenser Drum	N/A	170	1.4	Volume (m^3)	0.7
	Column III Condenser Drum	N/A	257	1.5	Volume (m^3)	22.6
Heat Exchangers	Cooler I	E-100	941	22.8	Cooler Duty (Btu/hr)	65,248,181.0
	Cooler II	E-101	336	8.3	Cooler Duty (Btu/hr)	6,187,920.2
	Cooler III	E-102	321	1.6	Cooler Duty (Btu/hr)	13,928,294.6
	Cooler IV	E-103	435	1.3	Cooler Duty (Btu/hr)	35,885,081.9
	Cooler V	E-104	180	2.0	Cooler Duty (Btu/hr)	152,703.3
Separators	Vapor Feed Separator	V-101	347	22.6	Volume (m^3)	3.4

Table 19: Equipment Summary Table for Feed TQ1

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