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Theoretical Ethylene Steam Cracking Plant Design and Techno-Economic Analysis

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Group 10

Executive Summary

In this report, a complete plant design for the production of 200 kta of ethylene ($900/MT) from ethane ($200/MT) has been completed up to Douglas Level 3 Hierarchy. 200 kta of ethylene is produced, with 14.3 kta of hydrogen ($1400/MT) as a valuable byproduct, in a plug flow reactor operating at 825 °C, 2 bar, and a .6 mole ratio of steam to ethane. The steam functions to prevent coking in the reactor, ensuring that the plant can run long term with no issues. Optimal conversion was calculated to be 66.3% from modeling in Aspen HYSYS utilizing the Soave Redlich-Kwong equation of state. This was achieved in a 10.87 m^3 plug flow reactor, with 277 tubes, each .05 meters in diameter and 20 meters long. The reactor effluent is fed to a cooler to stop reaction and to a separation system, producing 200 kta of ethylene, 14.3 kta of hydrogen, 31.7 kta of liquefied petroleum gas (LPG) and .8 kta of methane. The LPG and methane are used as fuel credit for the reactor to reduce heating costs, and all unreacted ethane is recycled. Utilizing this design, an NPV of $147.7 MM was achieved over the 15 year project, providing an IRR of 30% with a TCI of $215.2 MM. 0.67 kg CO_2 are produced per kg of ethylene, paid for by a $125 tax per metric ton of carbon dioxide sequestered. Additionally, the plant utilizes 83.0 MJ/kg ethylene produced. An economic analysis, along with a sensitivity analysis have determined that this plant is likely to be profitable, due to the low cost and minimal fluctuations in the price of ethane relative to the sale price of ethylene, such that ethylene prices can be dropped to $626/MT for the lifetime of the plant and the plant will remain profitable. As such, it is determined that further development of the ethylene plant is worth the cost.

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1 Introduction

1.1 Motivation and Background

The continued development of hydraulic fracturing and directional drilling in the United States has led to significant increases in the production of natural gas domestically. This gas contains more than 20% ethane, and as such ethane production in the United States has increased greatly. Because ethane is considered undesirable in most cases due to difficulties with transport, the demand and price remains low. This presents an opportunity for a plant to utilize ethane profitably, as low demand and high supply ensure a reliable supply with consistently low prices. The economic potential of this opportunity is especially high if designs for a plant and contracts can be locked in before any potential competitors, as increased demand would drive up construction and feed costs. BICC Inc. found a growing market for ethylene, with demand expected to outpace supply by at least 200 kta (2 million metric tons per year) within 2 years. Ethane contracts are currently available for $200/MT (metric ton), and ethylene currently sells at $900/MT, meaning there is economic potential for an ethylene plant with ethane as feed. Thus, BICC Inc. tasked our team with designing a 200 kta ethylene plant up to Level 3 in Douglas' Hierarchy[1]. An economic analysis was also performed, with optimizations for net present value (NPV) and investor rate of return (IRR) over a 15 year project life. As part of BICC Inc's aim for carbon neutrality, the cost of sequestering and storing all CO2 emissions was included in the analysis.

Additionally, due to advancements in separation technology, a pressure swing adsorption system (PSAS) can be used to produce high purity hydrogen as a valuable byproduct. Thus, the plant was designed both with and without hydrogen separation, with a comparison of profitability on both performed.

1.2 Market Analysis

While other options to produce ethylene are available, such as larger hydrocarbons (e.g. propane and butane) and naphthas, these chemicals already have alternative uses with greater demands, thus making them more expensive. It should be noted that ethane prices historically are volatile, with prices in 2018 spiking as high as $393/MT (Appendix D.1), and as low as $187/MT. While the current rate of $200 is not historically low, it is lower than the average historically, and still provides the opportunity for large profit margins for the production of ethylene. Because ethylene is the most produced organic chemical [2] in the world, with 150 million MT/year produced, the price of ethylene is resistant to market fluctuations, making it a reliable product.

1.3 Reaction Chemistry

The production of ethylene from ethane (Equation 1) occurs at very high temperatures, with our lab giving reaction data between 775 and 825 °C.

$$C_2H_6 \xrightleftharpoons{\Delta H_{rxn} = 136.27 \frac{kJ}{mol}} C_2H_4 + H_2 \tag{1}$$
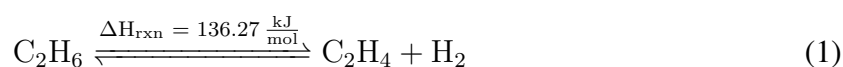
It also requires a significant heat duty to keep the product at operating temperature due to it being an extremely endothermic reaction. At these temperatures, side reactions of ethane are possible, producing longer chain hydrocarbons that lower the purity of the product and require

separation systems to remove. It is noted that the (Equation 1) forward and (Equation 2) will be the primary determinants of composition in the reactor effluent for low residence times, as the rate constants are multiple orders of magnitude greater than that of the (Equation 1) reverse and (Equation 2) (See AppendixB).

$$2\,C_2H_6 \xrightarrow{\Delta H_{rxn} = \text{-11.97 } \frac{kJ}{mol}} CH_4 + C_3H_8 \qquad (2)$$

$$C_2H_6 + C_2H_4 \xrightarrow{\Delta H_{rxn} = \text{-52.47 } \frac{kJ}{mol}} C_4H_{10} \qquad (3)$$
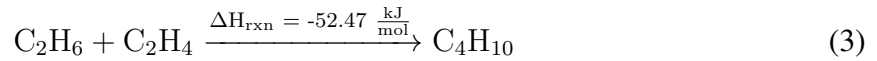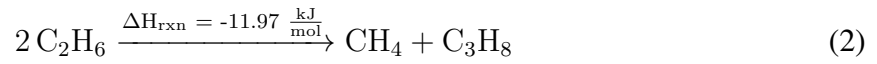
2 Conceptual Design

2.1 Process Overview

All Flow rates in kg/hr

Reactor Conditions
T= 825 C, P = 2 bar, MR = .6
11 m³

Fresh Feed Ethane
2.8x10⁴ kg/hr
25 C, 2 bar

Steam
1.5x10⁴ kg/hr
138 C, 2 bar

Mixer   Furnace   PFR   Cooler   Separation System

Reactor Inlet 5.7x10⁴ kg/hr
825 C, 2 bar

Reactor Outlet 5.7x10⁴ kg/hr

Ethylene 2.3x10⁴ kg/hr, -90 C, 2 bar
LPG 3.6x10³ kg/hr, -60 C, 2 bar
Waste Water 1.5x10⁴ kg/hr, 100 C, 2 bar
Methane 1.2x10² kg/hr, -200 C, 1 bar
Hydrogen 1.6x10⁵ kg/hr, -200 C, 10 bar

Recycle Ethane
1.4x10⁴ kg/hr
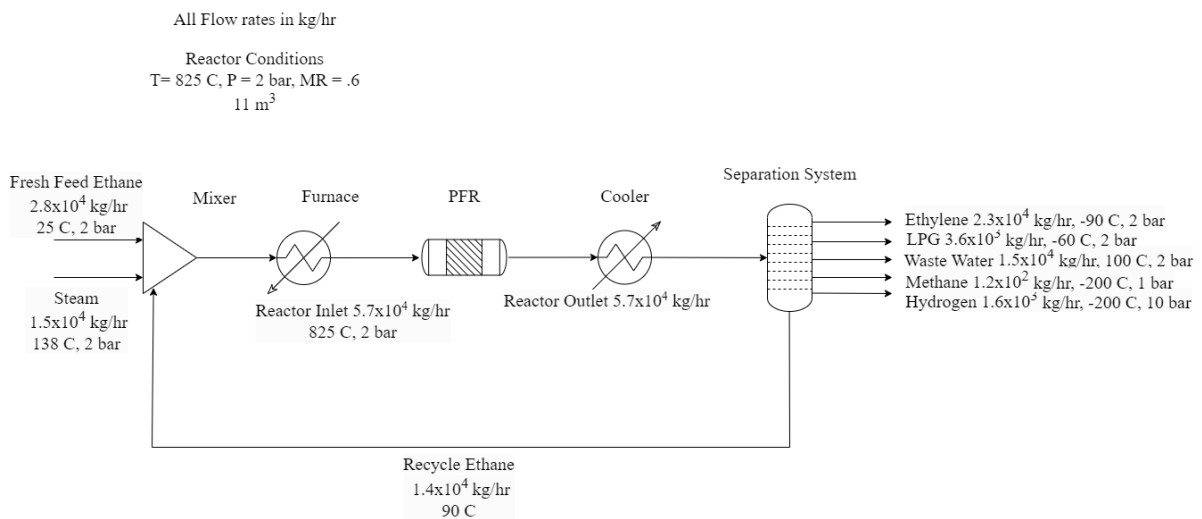90 C

Figure 1: Process flow diagram of thermal steam cracking of ethane.

Table 1: Process stream labels and specifications

Name	Temperature (°C)	Pressure (bar)	Molar Compositions	Mass Flow Rate (kg/hr)
Fresh Feed Ethane	25	2.0	1.0 C_2H_6	$2.8 * 10^4$
Steam	138	2.0	1.0 Steam	$1.5 * 10^4$
Recycle Ethane	-90	2.0	1.0 C_2H_6	$1.4 * 10^4$
Heater Inlet	78	2.0	0.62 C_2H_6, 0.38 Steam	$5.7 * 10^4$
Reactor Inlet	825	2.0	0.62 C_2H_6, 0.37 Steam	$5.7 * 10^4$
Reactor Outlet	825	2.0	0.15 C_2H_6, 0.28 Steam, 0.27 C_2H_4, 0.29 H_2, $1.1 * 10^{-5}$ CH_4, $1.1 * 10^{-5}$ C_3H_8, $2.0 * 10^{-2}$ C_4H_{10}	$5.7 * 10^4$
Water Separation	100	2.0	0.15 C_2H_6, 0.28 Steam, 0.27 C_2H_4, 0.29 H_2, $1.1 * 10^{-5}$ CH_4, $1.1 * 10^{-5}$ C_3H_8, $2.0 * 10^{-2}$ C_4H_{10}	$5.7 * 10^4$
Waste Water	100	2.0	1.0 H_2O	$1.5 * 10^4$
Hydrogen and Hydrocarbons	100	2.0	0.21 C_2H_6, 0.37 C_2H_4, 0.40 H_2, $1.5 * 10^{-5}$ CH_4, $1.5 * 10^{-5}$ C_3H_8, $2.8 * 10^{-2}$ C_4H_{10}	$4.2 * 10^4$
LPG Fuel	-60	2.0	$5.0 * 10^{-4}$ C_3H_8, 0.99 C_4H_{10}	$3.6 * 10^3$
Combined Gas	-60	2.0	0.22 C_2H_6, 0.38 C_2H_4, 0.41 H_2, $1.5 * 10^{-5}$ CH_4	$3.9 * 10^4$
Product and Recycle	-120	2.0	0.36 C_2H_6, 0.64 C_2H_4,	$3.7 * 10^4$
PSA Feed	-120	2.0	0.99 H_2, $3.7 * 10^{-5}$ CH_4	$1.8 * 10^3$
Byproduct Hydrogen	-200	10	1.0 H_2	$1.6 * 10^3$
Methane Fuel	-200	1.0	0.99 H_2, $4.0 * 10^{-4}$ CH_4	$1.8 * 10^2$
Product Ethylene	-90	2.0	1.0 C_2H_4	$2.3 * 10^4$

Using the provided reaction data, flow rates in and out of the plant (Table 2) were defined via six mass balances (Appendix A.1). A degree of freedom analysis was performed, which stated three independent variables had to be defined (AppendixA.1). Selectivity one (S_1) and selectivity two (S_2) are defined as selectivity to ethylene and propane respectively, and product ethylene is specified at 200 kta, allowing plant flow rates to be calculated as function of selectivity.
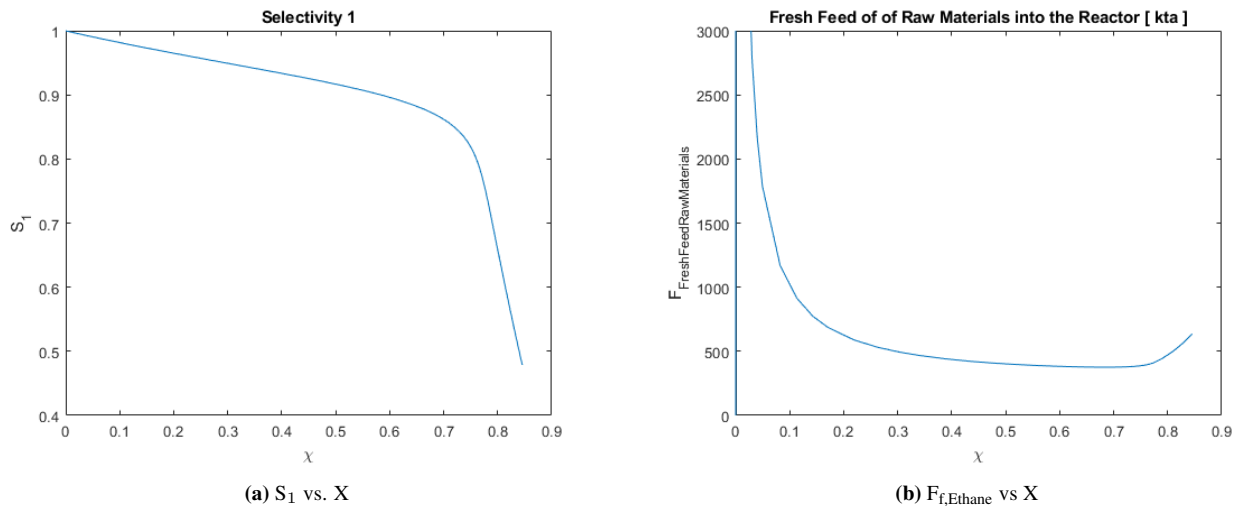

(a) S_1 vs. X

(b) $F_{f,Ethane}$ vs X

Figure 2: 2a provided an ideal range of single-pass conversion, defined as percent of ethane reacted in each pass of the reactor as seen in 2b
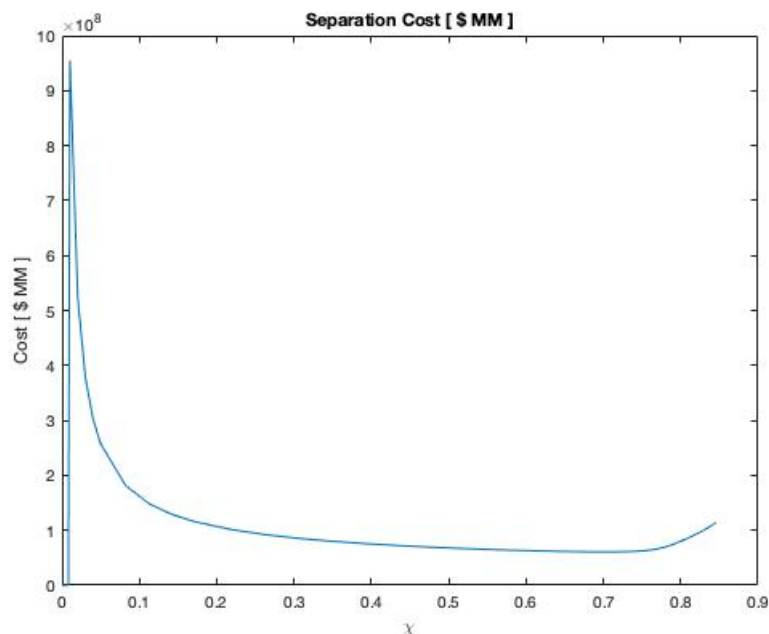
Figure 3: The cost of separation decreases as conversion increases. However, as illustrated in above as conversion exceeds 0.7 the cost of separation begins to increase.

Conversion of between 60% and 70% was considered the ideal range, as lower would require significant ethane recycle, driving heating and separation costs up significantly, while higher would increase rate of unwanted side reactions, lowering selectivity to the most valuable product of ethylene and its byproduct of hydrogen.

The process was designed with the assumption that the 245.3 kta of 99 mol% ethane feed can be assumed to be pure, and is fed to the plant as a pure liquid at 25 °C, thus requiring no extra processing before the feed. 134 kta of steam are also fed to the plant, as steam in the reactor helps to prevent coking and blocking in the tubing. The steam enters at 30 psia and 138 °C, and is fed to a mixer with the fresh and recycled ethane, such that the molar ratio of steam to ethane entering the reactor is 0.6. After the streams are combined, they are fed to a furnace that preheats the stream to 825 °C before entering the plug flow reactor (PFR). The PFR is designed with 277 tubes, each 0.05 meters in diameter, 20 meters long, and 10.87 m³ of total volume. The reactor is built with carbon steel, based on safe operating conditions from [3].

After exiting the reactor, the exit stream is immediately cooled to 100 °C so that pyrolysis stops quickly. The reactor effluent enters a separation system, where steam is removed as liquid water and sent to a waste water purification plant, all unreacted ethane is recycled to the plant, and the 31.7 kta stream of all hydrocarbons longer than ethane(LPG) are used as fuel for heating the reaction. The methane and hydrogen are sent to a pressure swing adsorption system, where 14.3 kta of 100 wt% hydrogen are sold as a byproduct and the remaining 0.8 kta of methane is used as fuel alongside the LPG stream. Finally, the 200 kta of ethylene, assumed to be separated at 100% purity, are sold as the primary product of the plant.

In addition to the equipment used in the plant towards producing ethane, a carbon capture system is also designed, used to sequester all carbon dioxide produced in the plant from burning fuel for heating the furnaces.

2.2 Energy Duty

The PFR was designed as an isothermal reactor due to the high combination of high reactor temperatures needed for the reaction and the primary reaction having a $\Delta H_{\text{rxn}} = +136.27 \frac{kJ}{mol}$, which will cause the temperature to rapidly decrease. As such, the feed stream had to be heated to the desired temperature of 825°C prior to entering the reactor, requiring a heat duty of 42.5 MW. A heat duty of 34.5 MW is also supplied to the reactor to ensure that the energy within the reactor stays constant at 825°C. This heat duty is equivalent to the net heat generation within the reactor, such that the combination of energy generated and energy supplied is zero, thus keeping the reactor isothermal. An additional energy cost comes from the separation of product streams, requiring a power of 212.8 MW to separate the reactor effluent stream into the desired product, recycle, and waste streams (Appendix C.3).

Table 2: Energy stream specifications

Name	Energy Flow (MW)
E-100	40
PFR-100	-40
E-101	40
X-100	-10
X-101	-5
X-102	-7
X-103	-1
X-104	4

Table 3: Equipment List

Equipment Name	Description	Size	Material	Duty (MW)
E-100	Fired Heater	N/A	Carbon steel[Perry's]	40
PFR-100	Plug Flow Reactor	11 m^3	Carbon steel	-40
Separation System	N/A	N/A	-20	-30

Table 4: Equipment Costs

Equipment Name	$MM
E-100	8.1
PFR-100	0.3
Separation System	61.4

2.3   Decision Variables and Design

Selectivity 1 vs. Conversion Changing Mole Ratio of Ethane to Steam

Legend:
- MR = 0.6
- MR = 0.7
- MR = 0.8
- MR = 0.9
- MR = 1.0
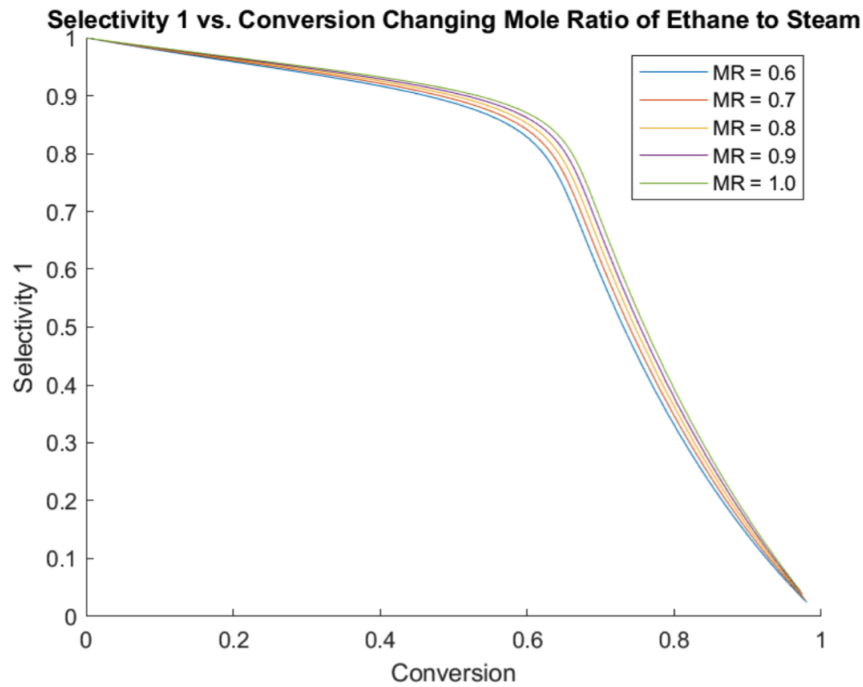
Figure 4: The above shows that the change in mole ratio is inconsequential towards selectivity and the cost to increasing the steam ratio outweighs the change in selectivity.

The mole ratio of steam to ethane entering the reactor was able to be varied from 0.6 to 1, and from Figure 5, which depicts the single pass conversion of the plant as a function of selectivity at different mole ratios of steam, it can be seen that less steam leads to better profitability. While more steam may lead to marginally higher selectivity towards ethylene in the reactor, the increased profit from better selectivity is negated by the drastically increased separation costs and waste water treatment due to the increased flow of water through the reactor.
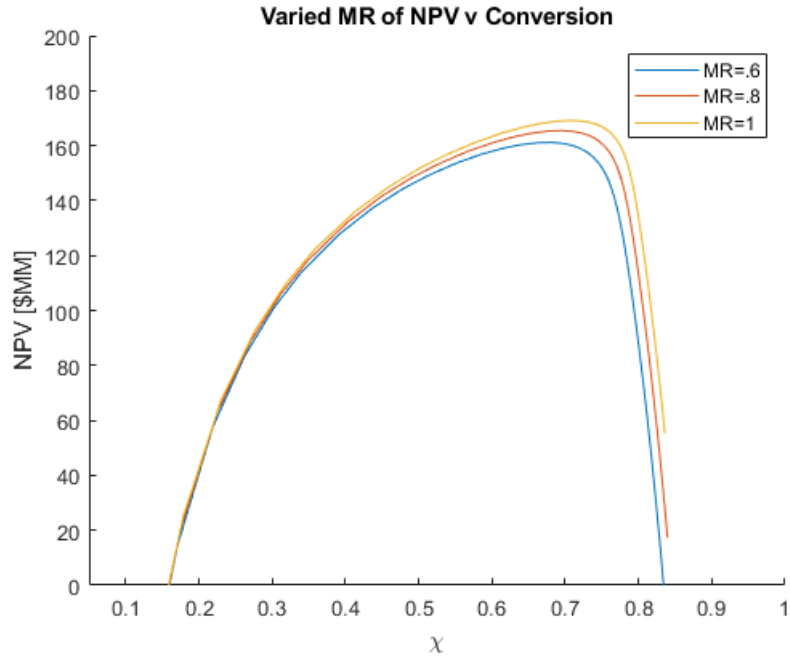
Figure 5: Plot of NPV vs. X with varying MR under constant P = 2 bar and T = 825°C.

By looking at the plot of conversion vs NPV in Figure 5, it is very clear that despite more steam giving better selectivity, its benefit is outweighed by making the system more expensive, as NPV does not increase significantly with mole ratio of steam. As such, when considering NPV, the optimal mole ratio of steam was found to be at the minimum of 0.6.
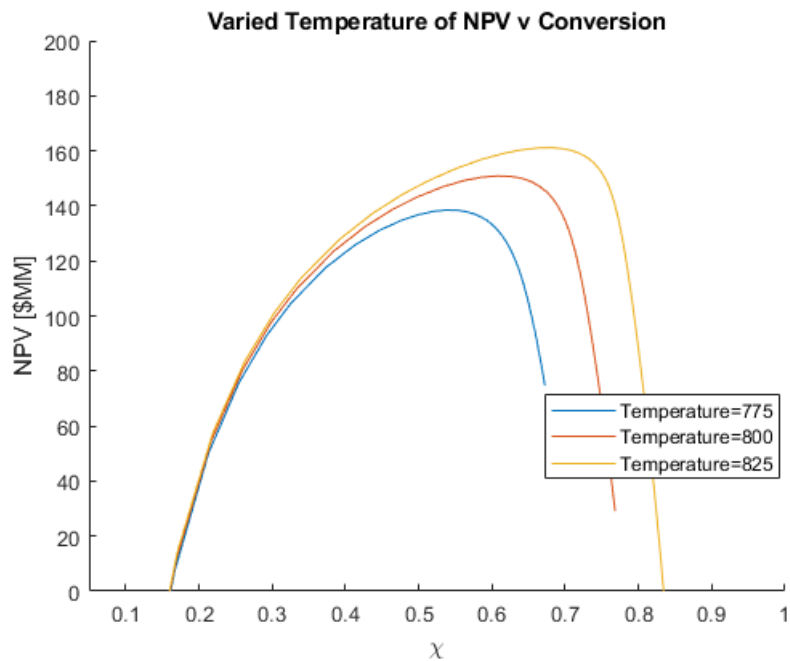
Figure 6: Plot of NPV vs. X with varying T under constant $P = 2$ bar and $MR = 0.6$.

The reactor temperature was able to be varied from 775°C to 825°C, and from Figure 6, it is shown that the optimal temperature of the reactor is 825°C, as it maximizes the NPV of the

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plant. This is a result of the rate constant for Equation (1) forward being strongly dependent on temperature, and as such increasing temperature increases the rate of reaction at any given volume, and reduces the selectivity towards other products. While Equation (2) may be more temperature sensitive than Equation (1) forward, it is limited by the concentration of ethylene in the reactor, and as long as residence times remain low, Equation (2) will not greatly reduce selectivity, and as such the highest temperature of 825°C maximizes the NPV of the plant.
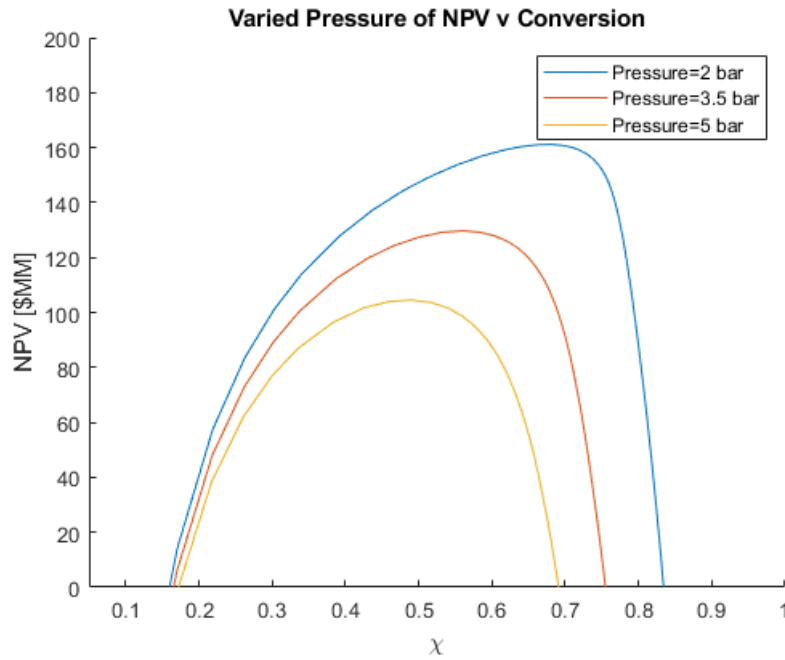
Figure 7: Plot of NPV vs. X with varying P under constant $T = 825°C$ and $MR = 0.6$.

The design variable with the greatest impact on NPV was reactor pressure, as seen from Figure 6. This is because low pressure will favor Equation (1) forward due to Equation (2) forward producing 2 moles of product for every mole of reactant consumed. Due to the impact of pressure on NPV, it is critical to operate at the lowest pressure in the range to maximize profitability for the plant.
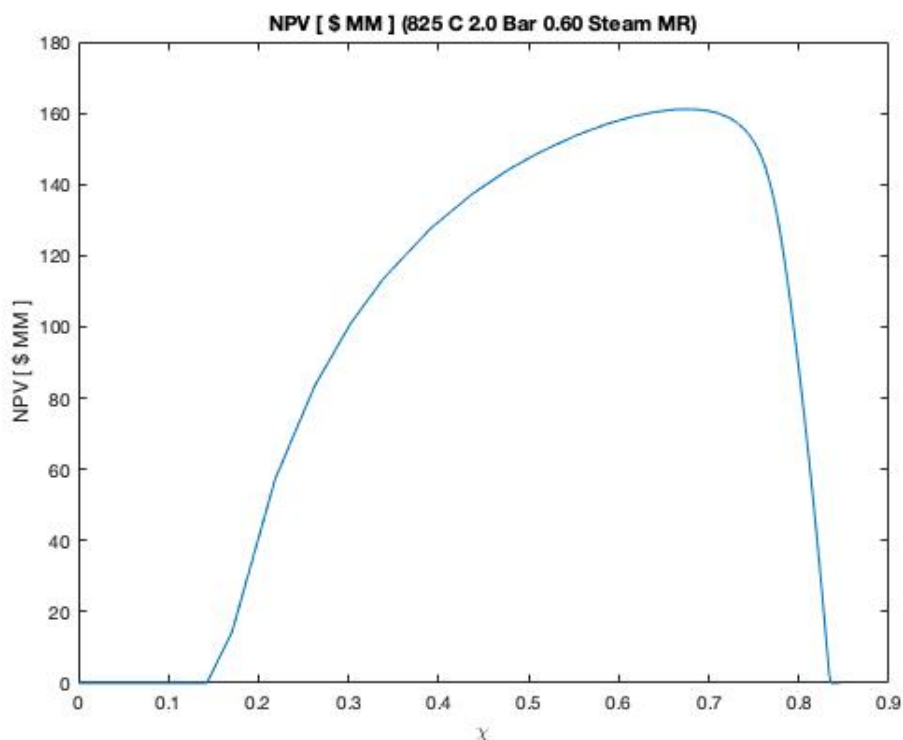
Figure 8: Plot of NPV vs. X. The above shows the optimal plant design corresponds to X = 0.6818.

By optimizing these variables in the reactor, S_1 was maximized such that even at high conversions, the production of unwanted byproducts like LPG and methane is minimized. This minimizes the feed cost by reducing the ethane needed to reach 200 kta of ethylene, reduces reactor cost by reducing the volume needed, reduces heating costs, and reduces separation costs by reducing the flow rate of reactor effluent as illustrated in Figure 7. All these in conjunction lead to NPV being increased from -$16 MM at the worst case variables up to $157 MM in the optimal conditions (See Appendix D For Cash Flowsheet).

2.4   Comparison With Aspen Model

Using the optimal reactor volume of 10.87 m³ and flow rates calculated at these conditions (Table E.2), a model was built in Aspen HYSYS V12.1, using the Soave-Redlich-Kwong (SRK) equation of state to model component interactions [4]. In order to reach the desired production rate of 200 kta of ethylene, which was adjusted to 208 kta in Aspen to account for 2 weeks of maintenance per year. This resulted in different flow rates and conversion in our model on Aspen when compared with the flow rates from Matlab. This can be attributed to differences in how intermolecular interactions were modeled, as our model was based off of the ideal gas law, while the Aspen model utilizes the SRK equation of state, more accurately modeling interactions between molecules at higher temperatures. As the reaction is taking place well above the critical temperatures of water and ethane, the Aspen model will be more accurate for modeling flow rates, and as such values from Aspen will be used for recommendations and calculations of profitability.

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3 Economic Analysis

Economic calculations were made using a 10 year straight line depreciation schedule, with assumptions of constant values for products, feed, and fuels. Additionally, estimates were used for outside battery loop costs and total capital investment based on the inside battery loop costs of the separation system, reactor, and furnace (See Appendix D).

3.1 Inside Battery Loop Costs and Yearly Cost of Operation
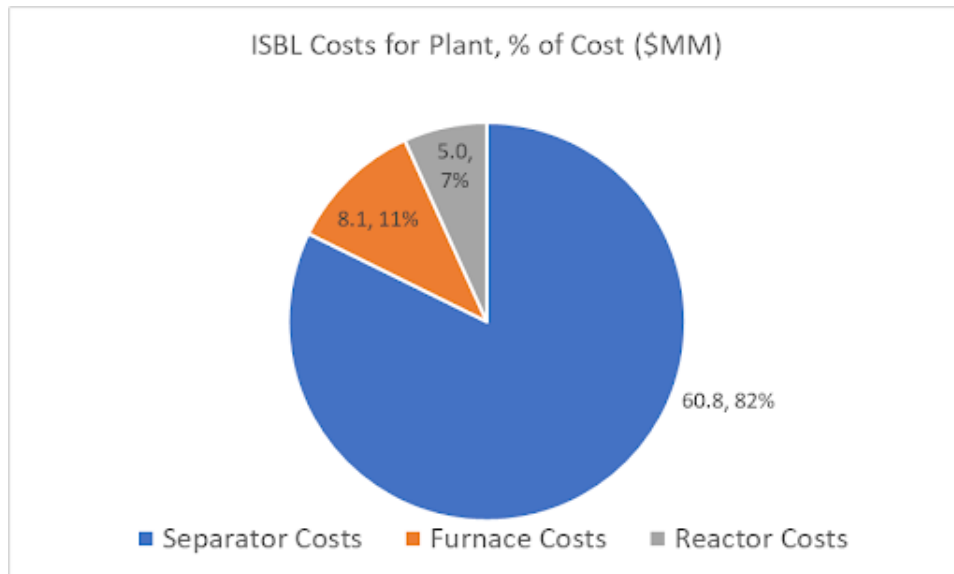
Figure 9: The above shows the ISBL breakdown for the plant, summing to $73.9 MM.

The ISBL costs were calculated based on estimates for separator costs using the work of mixing for fluids (C.3), and Douglas's Cost Correlations (C.3) for the cost of the furnace and reactor, giving a total ISBL of $74 MM, with the separation system consisting of 82% of the ISBL costs.

3.2 Total Capital Investment

The total capital investment for the plant was calculated using assumptions (See Appendix D) to convert the ISBL expenditures into the complete upfront cost of the plant, leading to a total capital investment of $215.2 MM, using the values seen below in Table 5.

Table 5: Total Fixed Capital Cost (TFCC).

Cost Type	$MM
ISBL	73.9
OSBL	29.6
Contingency Fee (CF)	25.9
Indirect Costs (IC)	38.8
TFCC	168.2
Working Capital (WC)	25.2
Start-up Costs (SC)	16.8
Land	5.0
TCI	215.2

3.3 Net Present Value Calculation
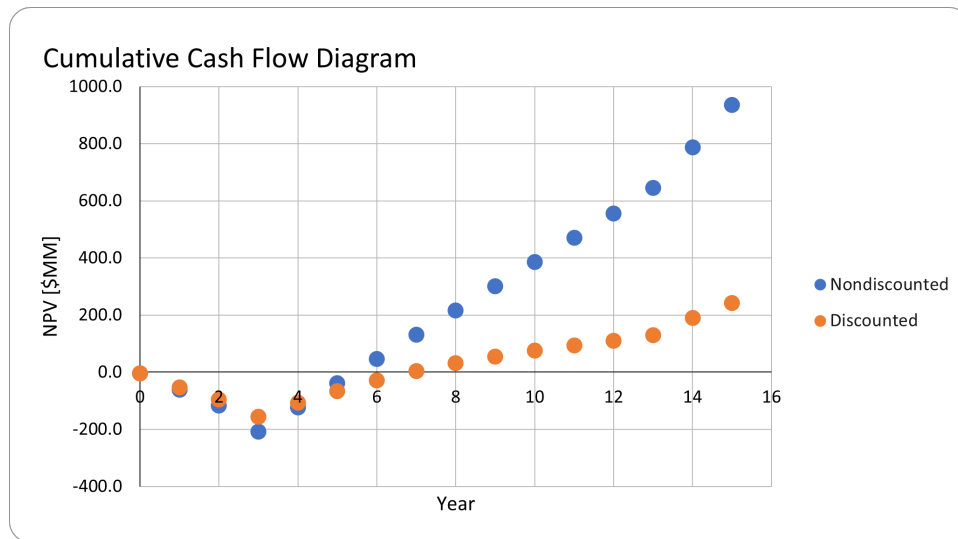
Figure 10: Cummulative cash flow in today's $ based on where costs are accrued at the end of the year.

Based on the NPV calculations in Excel and in Matlab, the NPV of the plant at year 15 is $147 MM, with an IRR of 30%. As seen in Figure 10, the break even point for the plant is year 7, including the 3 years of construction, resulting in 8 years of profitability for the expected project life of 15 years

3.4 Sensitivity Analysis
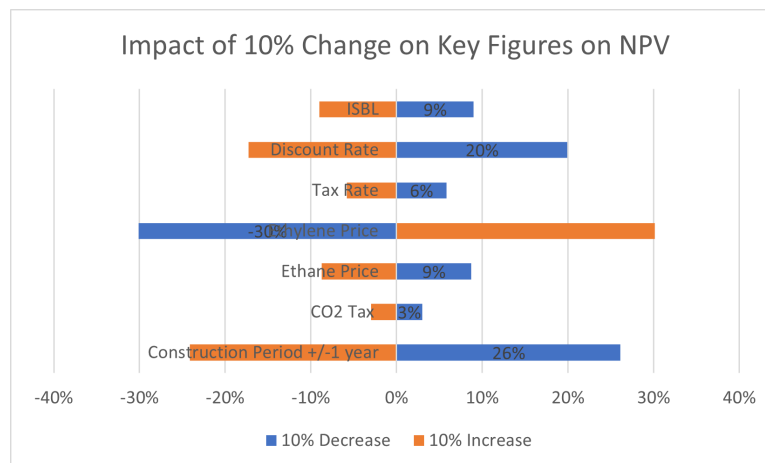
Figure 11: Tornado plot on the effect on NPV with changing parameters for plant based on 10% change in value. Construction period was changed by ± 1 year.

To determine the impact of different metrics on plant profitability, 6 metrics expected to have the largest impact on profitability were adjusted by $\pm 10\%$ to measure NPV response to changes. From the tornado plot above, it is clear that the plan is minimally impacted by changes in price of ethane, which is a good sign for a robust plant to offer long term profitability. It is vital that construction does not overrun however, as just a one year delay reduced the NPV by

24%. Changes in ethylene also had significant impacts on profitability, however this is both expected as it is the primary product, and unlikely, as ethylene is historically stable.

An analysis of the plants profitability was also completed for a recession, where the discount rate increased to 20% due to high uncertainty, both ethane and ethylene prices dropped 30% due to demand lowering. Finally, the construction period was increased to 5 years due to the impact of shortages and layoffs on build time (See Appendix D). This resulted in the NPV dropping to -\$17 MM. However, this proves the robustness of the plant's profitability, as it required a recession with impacts on prices that lasted for the full lifetime of the plant for the NPV to not be positive. The stability of the plant's profitability is also visible in the minimum sale price of ethylene, as in order to maintain positive NPV under normal assumptions, the price of ethylene can be dropped as low as \$630/MT, or 70% of the normal price of ethylene for the entirety of the project life.

4   Safety and Environmental Impact

Due to the high temperatures required for this process, there is an inherent risk with the operation of the plant. However, with proper training of staff, strong preventative safety practices, and efficient process control in the plant, these risks can be mitigated. The largest risk comes from the reactor, as the hydrogen and hydrocarbons are above their auto-ignition points for temperature, and as such without proper cooling outside the reactor, it is possible that reaction goes beyond desired conversion, leading to combustion of hydrocarbons in pipes not designed to handle it. To prevent this, the stream must be cooled right after reaction, and flow rates in the reactor must remain fast enough to keep conversion to hydrocarbons minimal. Full breakdown of safety hazards is present in the HAZOP section of Appendix E.

The environmental impact of the plant is mitigated by the carbon capture system implemented, helping keep the process carbon neutral. However, other impacts are present due to the feed being a product of hydraulic fracturing, and the extensive cleaning needed for water to be purified. Additionally, the process is producing 0.67 kg of CO2 per kg of ethylene, meaning that if the carbon capture system fails, there will be significant amounts of carbon dioxide released into the atmosphere.

5   Process Alternatives/Next Steps/Key Experiments Needed

An alternative plant was designed, with no separation of hydrogen and methane via PSA (PFD in Appendix F). Instead, the product stream was combusted in the plant as an energy source for the reactor and heater, thus reducing the separation costs and heating costs of the plant. However, this design was scrapped, as the total capital expense of the separator for all components is \$61 MM, and the sale of hydrogen increased the NPV of the plant by \$54 MM. Since the cost of separation is primarily determined by flow rates and desired exit composition, the cost of separation without the PSA will be far greater than \$7 MM , and thus the PSA is worth the additional cost upfront.

For further optimization of the plant, reaction rate data for higher temperatures and lower pressures is desired, as the optimal levels for both were at the maximum and minimum of the ranges given respectively. It is possible that the NPV of the plan can be further increased by operating at atmospheric pressure, or below, as this would push the equilibrium of pyrolysis of

ethane to ethylene even further towards the product. Likewise, increased temperatures could have the same effect due to the reaction being endothermic and reversible. The reactor and separation systems were modeled as isobaric for this design, which is likely not accurate, and pressure drops across the plant will need to be considered for higher level design to ensure that production of ethylene is not significantly impacted.

Furthermore, separation was assumed to be perfect for all but methane and hydrogen, as such for more accurate costs and revenues of products, lab scale separations must be completed to find both the efficiency of separating the components of the reactor effluent, as well as the energy duty required for separation to 99.9 mol% ethylene. Energy required for cooling, as well as the price of the heat exchanger network were not accounted for in Level 3 calculations, and to ensure the plant is profitable, these will need to be sized and priced to ensure that the impact on NPV is minimal.

6   Conclusions

An economic analysis of the Level 3 ethane steam cracking plant to produce ethylene shows that further development of the project is worthwhile. The project generates an NPV of $157 MM over its 15 year life time. Even with the significant assumptions made regarding costs, the sensitivity analysis of the plant proves the plant remains viable within normal variation of economic conditions, and that in order for the plant to become unprofitable, a very large recession must occur. As such, even with the significant assumptions made in regards to sizing and costing of equipment for the plant, it is likely that even as restrictions are put on the assumptions the plant will be capable of producing a highly positive NPV over the course of its lifetime.

7 References

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A Appendix

A.1 Level 1-3 Decisions and Mole Balances (Douglas Hierarchy)

Recall the system of reactions,

$$C_2H_6 \underset{}{\overset{\Delta H_{rxn} = 136.27 \frac{kJ}{mol}}{\rightleftharpoons}} C_2H_4 + H_2 \tag{A.1}$$

$$2\,C_2H_6 \xrightarrow{\Delta H_{rxn} = -11.97 \frac{kJ}{mol}} CH_4 + C_3H_8 \tag{A.2}$$

$$C_2H_6 + C_2H_4 \xrightarrow{\Delta H_{rxn} = -52.47 \frac{kJ}{mol}} C_4H_{10} \tag{A.3}$$
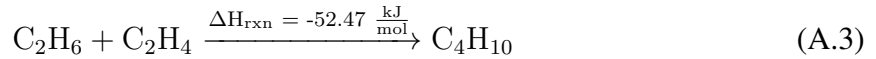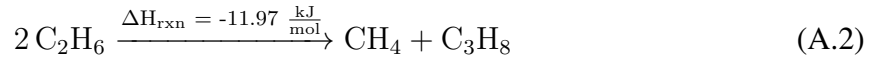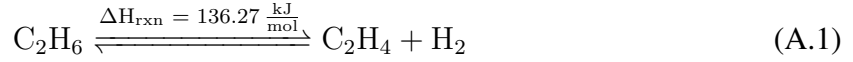
Using the above reactions, it can be determined the number of independent mole balances are $C - R = 6 - 3 = 3$, where C is the number of components and R is the number of reactions.

As such, the Level 2 mole balances using Douglas' Hierarchy of Design [1] and the systematic approach outlined by Doherty[5] can be written as follows:

Propane Mole Balance (same equation as methane balance):

$$-P_{C_3H_8} + 2F_{f,C_2H_6} = 0 \tag{A.4}$$

Butane Mole Balance:

$$-P_{C_4H_{10}} + F_{f,C_2H_6} = 0 \tag{A.5}$$

Hydrogen Mole Balance:

$$-P_{H_2} + F_{f,C_2H_6} = 0 \tag{A.6}$$

Ethane Mole Balance (assuming no ethane leaves the plant):

$$F_{f,C_2H_6} - P_{C_2H_4} - 2P_{C_3H_8} - P_{C_4H_{10}} = 0 \tag{A.7}$$

Ethylene Mole Balance:

$$-P_{C_2H_4} + F_{f,C_2H_6} - P_{C_4H10} = 0 \tag{A.8}$$

where P_i is the flow rate of species i in $\frac{mol}{s}$ leaving the plant and F_{f,C_2H6} is the flow rate of ethane into the plant in $\frac{mol}{s}$.

Subbing Equations (A.6) and (A.5) into Equation (A.8 gives our second independent mole

balance,

$$P_{C_2H_4} = P_{H_2} - P_{C_4H10} \tag{A.9}$$

Additionally, subbing Equations (A.4), (A.5), and (A.6) into (A.8) gives our final independent mole balance,

$$F_{f,C_2H_6} = P_{H_2} - 2P_{C3H8} - P_{C4H10} \tag{A.10}$$

Using a degree of freedom analysis DOF = V − E = 6 − 3, where V is the number of variables and E is the number of equations, there are 3 design specifications required. As defined in the problem statement, the production of ethylene is fixed, such that

$$P_{Ethylene} = 200 \tag{A.11}$$

(Note: $P_{Ethylene}[=]\frac{mol}{s}$ and must be converted to from kta to use these equations)

Since it is pivotal to understand the relationship between the desired product and the undesired product, two values of selectivity were defined as

$$S_1 = \frac{P_{Ethylene}}{F_{f,Ethane}} \tag{A.12}$$

$$S_2 = \frac{P_{Propane}}{F_{f,Ethane}} \tag{A.13}$$

Resolving the above species balances in terms of the design specifications (A.11), (A.12), and (A.13 results in the following:

$$F_{f,Ethane} = \frac{P_{Ethylene}}{S_1} \tag{A.14}$$

$$P_{Propane} = \frac{S_2}{S_1}P_{Ethylene} \tag{A.15}$$

$$P_{Methane} = \frac{S_2}{S_1}P_{Ethylene} \tag{A.16}$$

$$P_{Butane} = P_{Ethylene}\left(\frac{1}{2S_1} - \frac{S_2}{S_1} - \frac{1}{2}\right) \tag{A.17}$$

$$P_{Hydrogen} = P_{Ethylene}\left(\frac{1}{2S_1} - \frac{S_2}{S_1} + \frac{1}{2}\right) \tag{A.18}$$

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Now that the global plant balance has been accounted for, a closer examination of the internal streams should be evaluated. Proceeding with Douglas' Hierarchy[1], deliberate Level 3 Balance derivations for the recycle and reactor streams are conducted as follows:

Ethane Balance at the mixing point:

$$F_{f,Ethane} + R_{Ethane} = F_{Ethane} \tag{A.19}$$

Using another degree of freedom analysis DOF = $V - E = 3 - 1 = 2$, therefore we need 2 specifications. Since $F_{f,Ethane}$ is known from above, another design variable must be specified. In this case, the single-pass conversion can be written as $X = \frac{F_{Ethane} - R_{Ethane}}{F_{Ethane}}$ such that

$$R_{Ethane} = F_{Ethane}(1 - X) \tag{A.20}$$

Plugging Equation (A.20) into (A.19 dictates

$$F_{f,Ethane} + F_{Ethane}(1 - X) = F_{Ethane} \tag{A.21}$$

Finally, plugging in Equation (A.14) into Equations (A.21 and (A.20) gives the following,

$$F_{Ethane} = \frac{P_{Ethylene}}{S_1 X} \tag{A.22}$$

$$R_{Ethane} = \frac{P_{Ethylene}}{S_1}\left(\frac{1 - X}{X}\right) \tag{A.23}$$

B   Reaction Models, Rate Constants, and Calculated Design Variables

The final step to determine all the flow rates within the global envelope is to determine the flow rates of all species exiting the reactor system. The rates of reactions, rate constants, and reactor design equations are needed to generate a system of ODEs.[6] The rates of reaction are given by

$$r_1 = k_{1,f}[C_2H_6] - k_{1,r}[C_24][H_2] \tag{B.1}$$

$$r_2 = k_2[C_2H_6]^2 \tag{B.2}$$

$$r_3 = k_3[C_2H_6][C_2H_4] \tag{B.3}$$

where

$$k_{1,f} = 4.652 * 10^{13} \exp(\frac{-273,000}{RT}) \tag{B.4}$$

$$k_{1,r} = 9.91 * 10^{8} \exp(\frac{-173,800}{RT}) \tag{B.5}$$

$$k_{2} = 3.85 * 10^{11} \exp(\frac{-273,000}{RT}) \tag{B.6}$$

$$k_{3} = 7.083 * 10^{13} \exp(\frac{-252,000}{RT}) \tag{B.7}$$

(Note: $R[=]\frac{J}{mol*K}$, $T[=]K$, $E_A[=]\frac{J}{mol}$, $c_i[=]\frac{mol}{L}$, $k_{1,f}[=]\frac{1}{s}$, $k_{1,r}[=]\frac{L}{mol*s}$, $k_2[=]\frac{L}{mol*s}$)

The design equation for a PFR for i species is

$$\frac{dF_i}{dV} = r_i \tag{B.8}$$

Writing Equation (B.8) for each species and the total flow rate generates a system of ODEs, such that

$$\frac{dF_A}{dV} = -k_{1,f}c_A + k_{1,r}c_Bc_C - k_2c_A^2 - k_3c_Ac_B \tag{B.9}$$

$$\frac{dF_B}{dV} = k_{1,f}c_A - k_{1,r}c_Bc_C - k_3c_Ac_B \tag{B.10}$$

$$\frac{dF_C}{dV} = k_{1,f}c_A - k_{1,r}c_Bc_C \tag{B.11}$$

$$\frac{dF_D}{dV} = k_2c_A^2 \tag{B.12}$$

$$\frac{dF_E}{dV} = k_2c_A^2 \tag{B.13}$$

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$$\frac{dF_F}{dV} = k_3 c_A c_B \tag{B.14}$$

$$\frac{dF_{total}}{dV} = k_{1,f} c_A - k_{1,r} c_B c_C + k_2 c_A^2 - k_3 c_A c_B \tag{B.15}$$

where A = Ethane, B = Ethylene, C = Hydrogen, D = Methane, E = Propane, F = Butane

Since the reaction is operating as a gas phase PFR that calculates the molar flow rates, the concentrations, in molar concentrations, must be converted to the correct units. The gas system is assumed to follow the Ideal Gas Law, such that

$$c_i = \frac{F_i P_{total}}{F_{total} RT} \tag{B.16}$$

Plugging Equation (B.16) into the system of ODEs outputs the following:

$$\frac{dF_A}{dV} = -k_{1,f} \frac{F_A P_{total}}{F_{total} RT} + k_{1,r} \frac{F_B F_C P_{total}^2}{(F_{total} RT)^2} - k_2 \left(\frac{F_A P_{total}}{F_{total} RT}\right)^2 - k_3 \frac{F_A F_B P_{total}^2}{(F_{total} RT)^2} \tag{B.17}$$

$$\frac{dF_B}{dV} = k_{1,f} \left(\frac{F_A P_{total}}{F_{total} RT}\right) - k_{1,r} \frac{F_B F_C P_{total}^2}{(F_{total} RT)^2} - k_3 \frac{F_A F_B P_{total}^2}{(F_{total} RT)^2} \tag{B.18}$$

$$\frac{dF_C}{dV} = k_{1,f} \frac{F_A P_{total}}{F_{total} RT} - k_{1,r} \frac{F_B F_C P_{total}^2}{(F_{total} RT)^2} \tag{B.19}$$

$$\frac{dF_D}{dV} = k_2 \left(\frac{F_A P_{total}}{F_{total} RT}\right)^2 \tag{B.20}$$

$$\frac{dF_E}{dV} = k_2 \left(\frac{F_A P_{total}}{F_{total} RT}\right)^2 \tag{B.21}$$

$$\frac{dF_F}{dV} = k_3 \frac{F_A F_B P_{total}^2}{(F_{total} RT)^2} \tag{B.22}$$

$$\frac{dF_{total}}{dV} = k_{1,f} \frac{F_A P_{total}}{F_{total} RT} - k_{1,r} \frac{F_B F_C P_{total}^2}{(F_{total} RT)^2} + k_2 \left(\frac{F_A P_{total}}{F_{total} RT}\right)^2 - k_3 \frac{F_A F_B P_{total}^2}{(F_{total} RT)^2} \tag{B.23}$$

Given the ODE system of equations for the flow rates of each species out of the reactor, a basis inlet flow rate of Ethane is chosen arbitrarily to solve the system with respect to changing volume. This basis will later be scaled to the desired plant specifications. Given the flow rates into and out of the reactor give us the respective set of equations for conversion, selectivity to any product, and the residence time, τ,

$$X = \frac{F_A^0 - F_A}{F_A^0} \tag{B.24}$$

$$S_1 = \frac{F_B - F_B^0}{F_A^0 - F_A} \tag{B.25}$$

$$\tau = \frac{V}{q^0} = \frac{V P_{tot}}{RT \sum_{i=1}^c F_i^0} \tag{B.26}$$

where $q^0 = \frac{RT}{P_{tot}} \sum_{i=1}^c F_i^0$, and P_{tot} is the total pressure of the reactor, assuming isobaric and isothermal reaction.

Finally, using the global balances and internal recycle balance the true flow rates are used to scale the ODE solution accordingly to our specifications

$$V_{plant} = V \left(\frac{\sum_{i=1}^c (F_i^0)_{plant}}{\sum_{i=1}^c (F_i^0)} \right) \tag{B.27}$$

C Equipment Design Summary

C.1 Heater Design

The heater is designed to be adiabatic, so the amount of the energy that needs to be supplied is calculated by

$$\text{Installed Cost, \$} = \left(\frac{1800}{280} \right) (5.52 * 10^3) Q^{0.85} (1.27 + F_c) \tag{C.1}$$

where $Q = \Delta H_{rxn} \sum_{i=1}^c (F_i^0)_{plant}$ [=] $10^6 \frac{Btu}{hr}$ and $F_c = F_d + F_m + F_p = 1.10$ for Pyrolisis heater in carbon steel under 500 psi.[3]

C.2 Reactor Design and Installation Cost

The reactor is designed to be isothermal, therefore the amount of energy removed from the system is equal to the amount of heat added to the heater. The volume of the reactor was utilized to calculate the installed cost through the following correlation:

$$\text{Installed Cost,\$} = \left(\frac{1800}{280} \right) 101.9 D^{1.066} H^{0.82} (2.18 + F_c) \tag{C.2}$$

where $D = 0.5 * 3.2 = 1.6$ [=] ft [3], $H = \frac{V(D/2)^2(3.2)}{\pi}$ [=] ft, $F_c = F_{m,CS} + F_{p,CS} = 2.00$ [3]

C.3   Separation Cost

In following Douglas' Hierarchy, the evaluation of the separation system is detailed in Level 4; however, an approximation for cost of the separation system is required to properly evaluate the economics of the plant. Since the separation system is designed as a black box, therefore the minimum work, W_{min}, is used such that

$$W_{min} = \sum_{k=1}^{N}(F_k)RT\sum_{i=1}^{c}\left(x_i^k \ln\frac{x_i^k}{z_i}\right) + ... \tag{C.3}$$

where F_k is the flow rate of exiting stream k, x_i^k is the molar composition species i of exiting stream k, and z_i is the molar composition of the stream entering the separation system, for N streams. Equation (C.3) assumes constant temperature and pressure throughout the separation system. If a PSA system is added an additional term is added for the streams leaving the PSA system to account for the change in pressure, which is written as

$$W_{min} = \sum_{k=1}^{N-2}(F_k)... + RT\left[F_1\left(\ln\left(\frac{P_1}{P_f}\right) + x_i^1 \ln\frac{x_i^1}{z_i}\right) + F_2\left(\ln\left(\frac{P_2}{P_f}\right) + x_i^2 \ln\frac{x_2^1}{z_i}\right)\right] \tag{C.4}$$

where F_1 is the flow rate of the PSA overhead stream 1 $[=]\frac{mol}{s}$, P_1 is the PSA overhead pressure of stream 1, P_f is the pressure of the inlet stream to the PSA, x_i^1 is the overhead composition of species i of stream 1, and similar for the flow bottoms flow stream 2. The separation system operating expenses (OPEX) and capital expenses (CAPEX) are respectively calculated by

$$OPEX = \epsilon\lambda W_{min} \tag{C.5}$$

$$CAPEX = c(W_{real}) \tag{C.6}$$

where energy cost ϵ [=] $\frac{\$}{J}$, efficiency factor $\lambda = 50$, and capital cost correction factor c = 1 [=] $\frac{\$}{W}$. The combination of these installed and operating costs make up the ISBL costs.

D   Economic Assumptions, Formula, Spreadsheets

Table D.1: Economic Data

Substance	Price (value/cost)
Polymer–Grade Ethylene	$900/MT
Ethane	$200/MT
H2 (as a fuel) fuel value	$3.00/GJ
H2 (as a chemical)	$1,400/MT
Methane fuel value	$3.00/GJ
Propane fuel value	$3.00/GJ
Butane fuel value	$3.00/GJ
Natural Gas Fuel	$3.00/GJ
#2 Fuel Oil	$4.50/US gallon
Zeolite 5A sorbent for PSA	$5–25/kg
CO2 (low P, high nitrogen content)	$125/MT total outsource charge, see text
Process Steam	$6.84/GJ[5]
Waste Water & Other Waste Streams	[7]

In addition to the estimations for the separation costs, the economic assumptions in Tables (**??**) and (D.2) were used to calculate the TCI of the plant.

Table D.2: Assumptions for Total Fixed Capital Cost (TFCC). All values are in $MM

Cost	Assumptions
OSBL	0.4 (ISBL)
Contingency Fee (CF)	0.25 (ISBL + OSBL)
Indirect Costs (IC)	0.3 (ISBL + OSBL + Contingency Fee)
TFCC	OSBL + CF + IC
Working Capital (WC)	0.15 (TFCC)
Start-up Costs (SC)	0.1 (TFCC)
Land	5.0
TCI	TFCC + (WC + SC + Land)

After evaluating the capital costs, the following tables are used to evaluate the operating costs

Table D.3: Assumptions used to calculate VCOP in $\frac{\$MM}{yr}$

Revenue and Production Costs	Assumptions
Main Product Revenue (MPR)	$(F_{Ethylene})(Price_{Ethylene})$
Byproduct Revenue (BR)	$(F_{Hydrogen})(Price_{Hydrogen})$
Raw Materials Cost (COM)	$(F_{Ethane})(Price_{Ethane})$
Utilities Cost (UC)	$(F_{Steam})(Price_{Steam}) + (F_{LPG} + F_{Methane})(Price_{Fuel})$
CO$_2$ Sustainability Charge (CO$_2$ SC)	$[(F_{Methane} + F_{Propane} + F_{Butane})(Price_{Fuel})]\,\rho_{CO_2}$
VCOP	BR - COM + UC + (CO$_2$ SC)

where $F_i[=]\frac{MT}{yr}$ $Price_i[=]\frac{\$}{MT}$, $F_{Fuel}[=]\frac{mol}{yr}$, $Price_{Fuel}[=]\frac{\$}{GJ}$, $\rho_{CO_2}[=]\frac{g_{CO_2}}{mol}$

Table D.4: Assumptions used to calculate FCOP in $\frac{\$MM}{yr}$

Fixed Production Costs	Assumptions
Interest Rate (IR)	0.15 (FCI)
Administrative Costs (AGS)	0.05 (Total Revenue)
FCOP	Interest + AGS

The plant was designed with a 15 year project life, and a 3 year construction schedule, with fixed capital evenly distributed across the three years. Working capital and start up costs were priced at year 3, and a 10 year straight line depreciation estimate was used to calculate depreciation. A 27% tax on taxable income, defined as gross profit minus depreciation, was used to calculate cash flow, and at the end of the project, the salvage value was assumed to be 5% of the FCI. The following two pages are the cash flow spreadsheets using the values from these assumptions and during a recession, respectively.

BICC, Inc.
123 Lagoon Road
Santa Barbara, CA

ECONOMIC ANALYSIS

Project Name: Ethylene Production via Ethane Cracking of Theramal Steam Group 10

Rev	Date	BY	APVD	Rev	Date	BY	APVD
V1.1	2/14/2023						
V2	3/13/2024	WJ	IH	TR	MFD	JPC	BY

Plant Location
Case Description

REVENUES AND PRODUCTION COSTS

	$MM/yr	
Main product revenue	180.0	Ethylene ($/MT * MT/yr)
Byproduct revenue	21.7	Hydrogen ($/MT * MT/yr)
Raw materials cost	49.5	Ethane ($/MT * MT/yr)
Utilities cost	0.3	Steam + Fuel
Consumables cost	0.0	
CO_2 sustainability charge	13.1	
VCOP	41.2	
Salary and overheads	0.0	
Maintenance	0.0	
Interest	15.0	
AGS	10.1	~5% Revenue
FCOP	25.1	

CAPITAL COSTS

	$MM	
ISBL Capital Cost	73.9	(Rxtr, Sep, He
OSBL Capital Cost	29.6	
Indirect Cost	38.8	
Contingency	25.9	
Total Fixed Capital Cost	168.2	
Working Capital	25.2	5%-30% FCI
Start-up Costs	16.8	~10%FCI
Land	5.0	
Total Capital Investment	215.2	

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% SU	% FCOP	% VCOP
0					
1	33%				
2	33%				
3	33%	100%	100%		
4				100%	100%
5				100%	100%
6+				100%	100%

ECONOMIC ASSUMPTIONS

On Stream	8400 hr/yr	Discount Rate	15%	Depreciation method	Straight-Line
	350 day/yr	Tax Rate	27%	Depreciation period	10 yrs
Project Life	15 yr	Salvage Value	5%		

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project Year	Cap. Ex.	Revenue	COM	Gr. Profit	Depren.	Taxable Inc	Taxes Paid	Cash Flow	Cummulative Cash Flow	PV of CF	Cummulative PV of CF	NPV
0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	-5.0	-5.0	-5.0	-5.0	-5.0
1	55.5	0.0	0.0	0.0	0.0	0.0	0.0	-55.5	-60.5	-48.3	-53.3	-53.3
2	55.5	0.0	0.0	0.0	0.0	0.0	0.0	-55.5	-116.0	-42.0	-95.2	-95.2
3	97.5	0.0	0.0	0.0	0.0	-17.7	-4.8	-92.8	-208.8	-61.0	-156.2	-156.2
4	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	-121.0	50.2	-106.0	-106.0
5	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	-33.3	43.6	-62.4	-62.4
6	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	54.5	37.9	-24.5	-24.5
7	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	142.2	33.0	8.5	8.5
8	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	230.0	28.7	37.2	37.2
9	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	317.7	24.9	62.1	62.1
10	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	405.5	21.7	83.8	83.8
11	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	493.2	18.9	102.7	102.7
12	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	581.0	16.4	119.1	119.1
13	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	673.7	14.3	138.3	133.3
14	0.0	180.0	66.3	113.7	17.7	96.0	25.9	87.7	817.0	12.4	199.0	145.7
15	-8.4	180.0	66.3	113.7	17.7	96.0	25.9	96.2	968.6	11.8	252.8	157.6

ECONOMIC ANALYSIS

NPV	15 years	157.6	$MM
NPV at yr	15	11.8	$MM
IRR		31%	

NOTES

1. All cash flows are assumed to occur at the end of the project year.
2.
3.

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ECONOMIC ANALYSIS

Project Name: Ethylene Production via Ethane Cracking of Theramal Steam Group 10

Rev	Date	BY	APVD	Rev	Date	BY	APVD
V1.1	2/14/2023	JPC	MFD				
V2	3/13/2024	IH	WJ	TR			

Plant Location
Case Description

REVENUES AND PRODUCTION COSTS

	$MM/yr	
Main product revenue	126.0	Ethylene ($/MT * MT/yr)
Byproduct revenue	21.7	Hydrogen ($/MT * MT/yr)
Raw materials cost	34.7	Ethane ($/MT * MT/yr)
Utilities cost	0.3	Steam + Fuel
Consumables cost	0.0	
CO_2 sustainability charge	16.9	
VCOP	30.2	
Salary and overheads	0.0	
Maintenance	0.0	
Interest	15.0	
AGS	7.4	~5% Revenue
FCOP	22.4	

CAPITAL COSTS

	$MM	
ISBL Capital Cost	73.9	(Rxtr, Sep,)
OSBL Capital Cost	29.6	
Indirect Cost	38.8	
Contingency	25.9	
Total Fixed Capital Cost	168.2	
Working Capital	25.2	5%-30% FC
Start-up Costs	16.8	~10%FCI
Land	5.0	
Total Capital Investment	215.2	

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% SU	% FCOP	% VCOP
0	0%				
1	20%				
2	20%				
3	20%				
4	20%				
5	20%	100%	100%		
6+				100%	100%

ECONOMIC ASSUMPTIONS

On Stream	8400 hr/yr	Discount Rate	20%
	350 day/yr	Tax Rate	27%
Project Life	15 yr	Salvage Value	5%
		Depreciation method	Straight-Line
		Depreciation period	10 yrs

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project Year	Cap. Ex.	Revenue	COM	Gr. Profit	Depcn.	Taxable Inc	Taxes Paid	Cash Flow	Cummulative Cash Flow	PV of CF	Cummulative PV of CF	NPV
0	5.0	0.0	0.0	0.0	0.0	0.0	0.0	-5.0	-5.0	-5.0	-5.0	-5.0
1	33.6	0.0	0.0	0.0	0.0	0.0	0.0	-33.6	-38.6	-28.0	-33.0	-33.0
2	33.6	0.0	0.0	0.0	0.0	0.0	0.0	-33.6	-72.3	-23.4	-56.4	-56.4
3	33.6	0.0	0.0	0.0	17.7	-17.7	-4.8	-28.9	-101.1	-16.7	-73.1	-73.1
4	33.6	0.0	0.0	0.0	17.7	-17.7	-4.8	-28.9	-130.0	-13.9	-87.0	-87.0
5	75.7	0.0	0.0	0.0	17.7	-17.7	-4.8	-70.9	-200.9	-28.5	-115.5	-115.5
6	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	-142.5	19.5	-96.0	-96.0
7	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	-84.2	16.3	-79.7	-79.7
8	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	-25.8	13.6	-66.1	-66.1
9	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	32.6	11.3	-54.8	-54.8
10	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	90.9	9.4	-45.4	-45.4
11	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	149.3	7.9	-37.5	-37.5
12	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	207.7	6.5	-31.0	-31.0
13	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	271.0	5.5	-20.5	-25.5
14	0.0	126.0	52.6	73.4	17.7	55.8	15.1	58.4	363.0	4.5	12.1	-21.0
15	-8.4	126.0	52.6	73.4	17.7	55.8	15.1	66.8	463.4	4.3	39.8	-16.6

ECONOMIC ANALYSIS

NPV	15 years	-16.6 $MM
NPV at yr	15	4.3 $MM
IRR		17%

NOTES

1. All cash flows are assumed to occur at the end of the project year.
2.
3.

E   Safety

E.1   Safety Data Sheet

Table E.1: Safety precautions for plant chemicals

Species	Flammability	Explosive Limits	Toxicology	Corrosiveness
Ethane	Extremely flammable gas (Category 1) Auto-ingition Temperature 287 °C Flash point: -104 °C	Upper explosion limit: 8.4% Lower explosion limit: 1.8%	TLV: 1000 ppm 8 hours Normally stable, even under fire conditions	Mild skin irritant Respiratory irritant
Ethylene	Extremely flammable gas (Category 1) Auto-ingition Temperature 450 °C Flash point: -136 °C	Upper explosion limit: 36% Lower explosion limit: 2.7%	TLV: 200 ppm 8 hours	Ingestion: nervous system depression Inhalation: nausea and dizziness Dermal: frostbite
Hydrogen	Extremely flammable gas (Category 1) Auto-ingition Temperature 560 °C Flash point: -104 °C	4 - 77 vol%	Simple asphyxiant	Mild skin irritant May react violently with oxidants
Methane	Extremely flammable gas (Category 1) Auto-ingition Temperature 537 °C Flash point: -104 °C	Upper explosion limit: 14% Lower explosion limit: 5%	TLV: 1000 ppm 8 hours	Eye contact: burns/frostbite Skin contact: burns/frostbite
Propane	Extremely flammable gas (Category 1) Auto-ingition Temperature 287 °C Flash point: -104 °C	Upper explosion limit: 8.4% Lower explosion limit: 1.8%	TLV: 1000 ppm 8 hours	Dermal: burns/frostbite Inhalation: may cause rapid suffocation May form explosive mixtures with air
Butane	Extremely flammable gas (Category 1) Auto-ingition Temperature 287 °C Flash point: -60 °C	Upper explosion limit: 8.5% Lower explosion limit: 1.9%	TLV: 1000 ppm 8 hours	Dermal: frostbite Inhalation: nausea and dizziness May form explosive mixtures with air

E.2   Preliminary HAZOP

Item	Parameter	Guide word	Cause	Consequence	Safeguards	Recommendation
Furnace	Ethane Flow	More	Valve open	Higher ethane-to-steam ratio could lead to coking causing pressure build-up leading to explosion	Valve controller	Fail-close valve to stop heat flow going into heater
		Less	Valve closed/leak	Ethane is overheated causing greater risk of auto-ignition	Temperature controller	At high temperatures flood heater with steam
	Steam Flow	Less	Valve closed/leak	Increased risk of side reactions, higher pressure and temperature, increasing risk of explosion	Valve controller	Fail-open valve
	Temperature	More	Fuel valve open	Higher risk of combustion	Temperature controller	Fail-close valve
	Pressure	More	Coke build-up	Decreased volume in reactor, leads to increased pressure and risk of explosion	Pressure guage linked to pressure release valve	Recommended consistent checks on the stream pressure. Regular checks to clean pipes
Mixer	Fresh Ethane Flow	More	Valve Open	Too much Ethane in feed, coking and potential autoignition	Valve controller	Fail-close valve
		Less	Pipe leak	Chemical released in air causes increased risk of auto-ignition and inhalation	Chemical detector	Consistent checks on chemical detectors. Nearby staff leave area to prevent inhalation
	Recycle Ethane Flow	More	Impurities In separation	Impurities in recycle lead to potential reactor coking and pressure build-up, explosion	Purge stream from recycle to prevent build up of any chemical	Extra testing on separation systems prior to operation, implement purge if necessary
		Less	Pipe leak	Chemical released in air causes increased risk of auto-ignition and inhalation	Chemical detector	Consistent checks on chemical detectors. Nearby staff leave area to prevent inhalation
	Steam Flow	Less	Pipe leak	Burn risk to plant workers if in vicinity of pipe venting hot steam. Increased risk of side reactions, higher pressure and temperature, increasing risk of explosion	Safety training for employees	Increase flow rate of steam to ensure safe operation in reactor
PFR	Inlet Flow	Less	Valve closed/leak	Ethane is overheated causing greater risk of auto-ignition	Temperature controller	At high temperatures flood heater with steam
	Outlet Flow	Less	Reactor Blockage	Flow out less than flow in leads to pressure build up, possible reactor explosion if left too long	Pressure gauge linked linked to pressure release valve	Consistent checks on reactor pressure, ensure no changes in operating with time
	Pressure	More	Coke build-up	With enough pressure build up, can lead to explosion in reactor if allowed enough time	Pressure gauge linked linked to pressure release valve	Consistent checks on reactor pressure, ensure no changes in operating with time
		Less	Leak in Pipe	Chemical released in air causes increased risk of auto-ignition and inhalation	Chemical detector	Consistent checks on chemical detectors. Nearby staff leave area to prevent inhalation
	Temperature	More	Too much power to furnace	Too much fuel can lead to surpassing safe limits of reactor temperature, resulting in reactor failure	Temperature controller	Fail-close valve on furnace fuel
Cooler	Inlet Flow	More	Valve Open	Stream does not fully cool, thus does not fully seperate in separation system, impurities in recycle lead to potential reactor coking and pressure build-up, explosion	Purge stream from recycle to prevent build up of any chemical	Fail close valve
		Less	Leak in Pipe	Chemical released in air causes increased risk of auto-ignition and inhalation	Chemical detector	Consistent checks on chemical detectors. Nearby staff leave area to prevent inhalation
	Outlet Flow	More	Valve Open	Insufficiently cooled separator feed, resulting in less pure product and recycle streams and potential accumulation of waste in system	Temperature controller	Fail close valve
		Less	Steam cools to water	Pressure drop in pipes, potential blocking in pipes from liquid getting stuck	Temperature controller	Piping between cooler and separator angled downwards to prevent any potential liquid from going backwards, instead will flow into separator system
	Pressure	More	Build up of impurity in cooler	Can lead to blockage and damage to cooler	Pressure gauge linked to pressure release valve	Regular checks on condenser, ensure no build up of residue inside
		Less	Steam cools to water	Pressure drop in pipes, potential blocking in pipes from liquid getting stuck	Temperature controller	Piping between cooler and separator angled downwards to prevent any potential liquid from going backwards, instead will flow into separator system
	Temperature	More	Valve Open, flows too fast through	Insufficiently cooled separator feed, resulting in less pure product and recycle streams and potential accumulation of waste in system	Valve controller	Fail close valve

Separation System	Inlet Flow	Less	Heat exchanger fluid too cold	Potential for liquid to from before separator, resulting in build up in pipes	Temperature controller	Piping between cooler and separator angled downwards to prevent any potential liquid from going backwards, instead will flow into separator system
		More	Valve open	Too fast flow in separators results in imperfect separations, causes impurities in recycle stream and potential accumulation of mass	Valve controller	Fail close valve
		Less	Steam condenses to water in pipe after cooler	Pressure drop in pipes, potential blocking in pipes from liquid getting stuck	Temperature controller	Piping between cooler and separator angled downwards to prevent any potential liquid from going backwards, instead will flow into separator system
		Less	Leaks in system	Chemical released in air causes increased risk of auto-ignition and inhilation	Chemical detector	Consistent checks on chemical detectors. Nearby staff leave area to prevent inhilation
	Pressure	More	Build up of impurity in separator (large hydrocarbons)	Can cause blocking in separator, leading to less ideal separation and impurities in feed, recycle leading to accumulation of mass over time	Pressure Sensor Connected to Pressure release valve	Testing of reactor effluent composition at lab scale to check that large hydrocarbons that can form do not cause blockages over long term plant life
		Less	Leaks in system	Chemical released in air causes increased risk of auto-ignition and inhilation	Chemical detector	Consistent checks on chemical detectors. Nearby staff leave area to prevent inhilation
	Temperature	More	Cooler Failure	High temperatures make separating components more difficult due to very close boiling points, results in bad separation and accumulation in system due to recycle	Temperature Controller separator system	Fail close valve

F Aspen HYSYS Simulation vs. MATLAB Conceptual Design

Table E.2: MATLAB Process stream labels and specifications

Name	Temperature (°C)	Pressure (bar)	Molar Compositions	Mass Flow Rate (kg/hr)
Fresh Feed Ethane	25	2.0	1.0 C_2H_6	$4.1 * 10^4$
Steam	138	2.0	1.0 Steam	$7.9 * 10^3$
Recycle Ethane	-100	2.0	1.0 C_2H_6	$1.3 * 10^4$
Heater Inlet	78	2.0	0.87 C_2H_6, 0.13 Steam	$6.2 * 10^4$
Reactor Inlet	825	2.0	0.87 C_2H_6, 0.13 Steam	$6.2 * 10^4$
Reactor Outlet	825	2.0	0.08 C_2H_6, 0.30 Steam, 0.20 C_2H_4, 0.31 H_2, $5.4 * 10^{-5}$ CH_4, $5.4 * 10^{-5}$ C_3H_8, 0.1 C_4H_{10}	$6.2 * 10^4$
Water Separation	100	2.0	0.08 C_2H_6, 0.30 Steam, 0.20 C_2H_4, 0.31 H_2, $5.4 * 10^{-5}$ CH_4, $5.4 * 10^{-5}$ C_3H_8, 0.1 C_4H_{10}	$6.2 * 10^4$
Waste Water	100	2.0	1.0 H_2O	$7.9 * 10^3$
LPG Fuel	-100	2.0	N/A	N/A
Byproduct Hydrogen	-100	10	1.0 H_2	N/A
Methane Fuel	-100	1.0	0.99 H_2, $4.0 * 10^{-4}$ CH_4	N/A
Product Ethylene	-100	2.0	1.0 C_2H_4	$2.3 * 10^4$
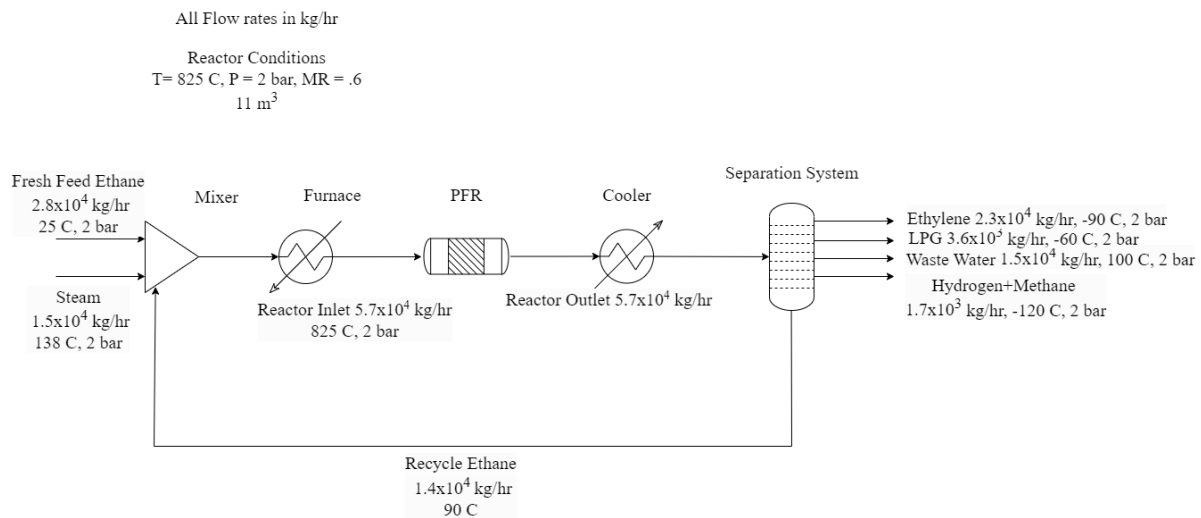
Figure E.1: Process flow diagram of thermal steam cracking of ethane without PSA system.

G Additional MATLAB Generated Figures
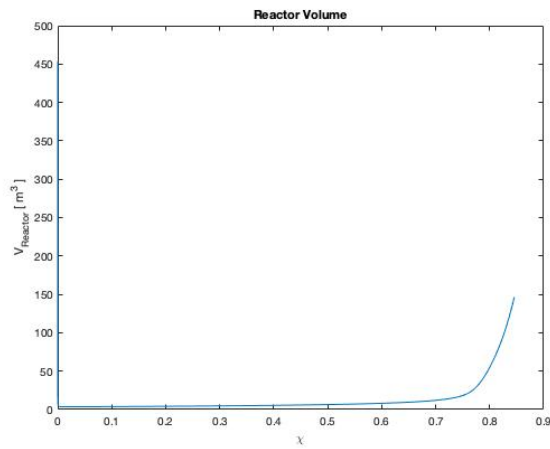
(a) Reactor Volume vs Conversion
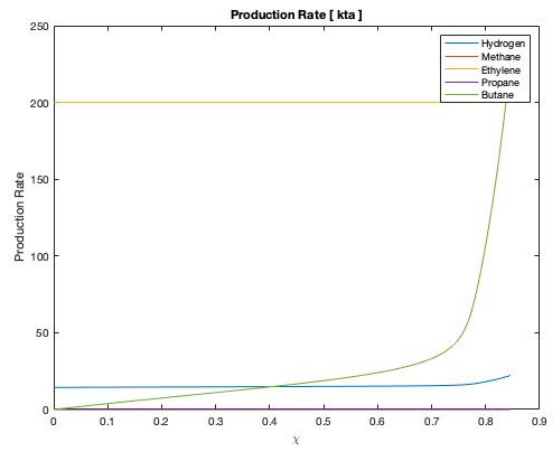
(b) Production Rate vs Conversion
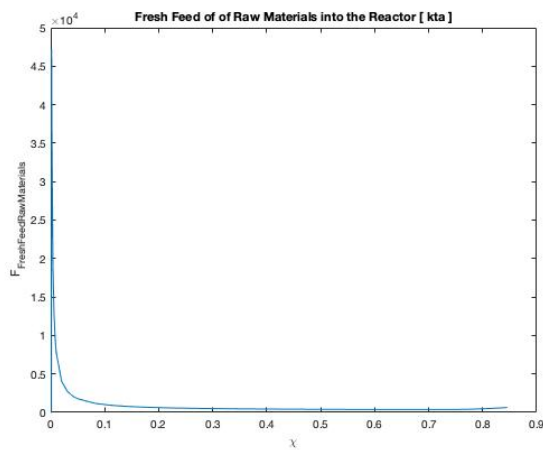
(a) Fresh Feed of Raw Materials vs Conversion

(b) Recycle of Ethane Flow Rate vs Conversion

Figure F.4: Composition of flow entering separation system
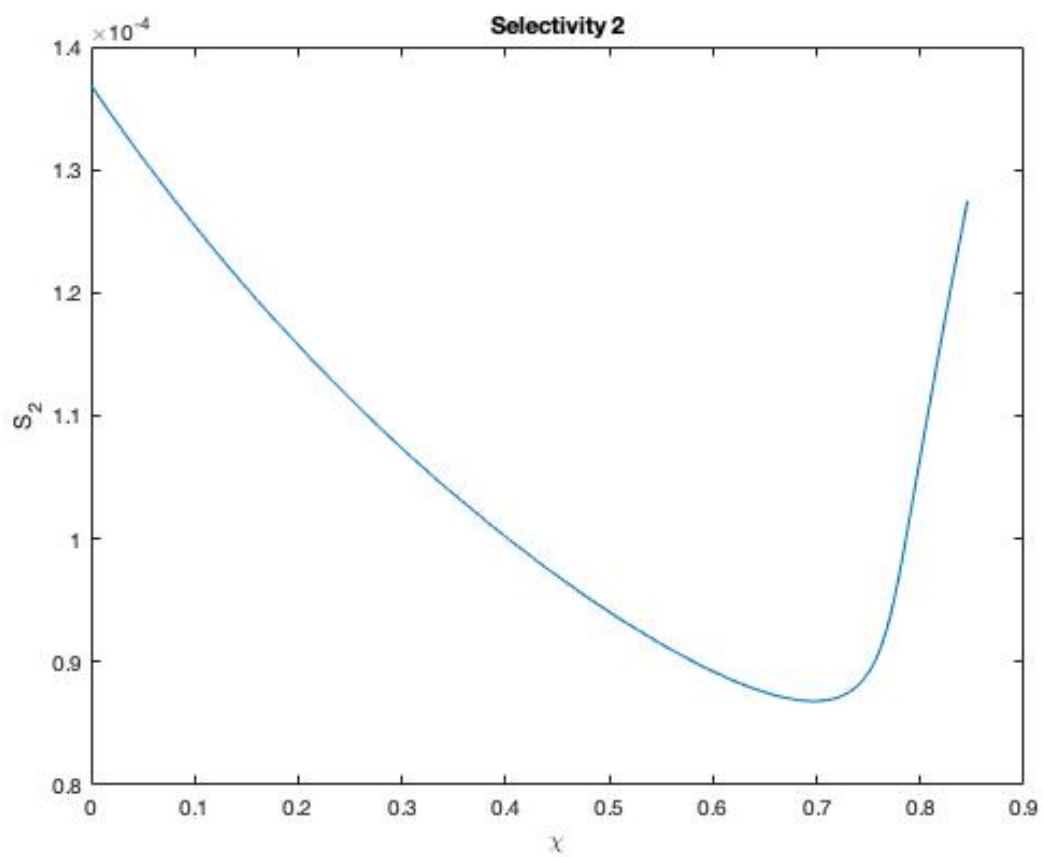
Figure F.5: Selectivity 2 vs Conversion
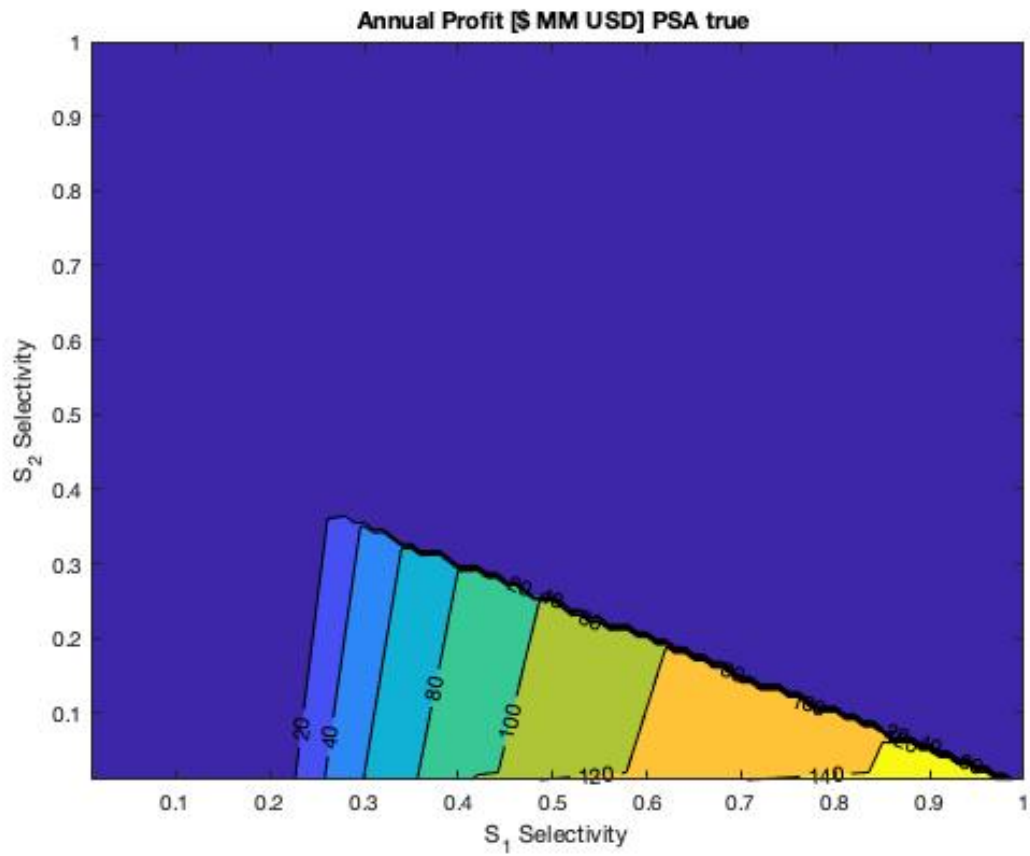
Figure F.6: Level 2: Economic Potential vs Selectivies 1 and 2

H Commented Matlab Code

```matlab
  1
  2 % Clear the console
  3 clc;
  4 % Close all the windows
  5 close all;
  6 % Clear Workspace Variables
  7 clear;
  8
  9 global S1_MIN S1_MAX S1_POINTS;
 10 global S2_MIN S2_MAX S2_POINTS;
 11 global INVALID_FLOWRATE;
 12 global Fethyl_S1S2_plotOpt;
 13 global MT_PER_KT G_PER_KT GJ_PER_KJ;
 14 global VALUE_ETHANE VALUE_ETHYLENE VALUE_HYDROGEN_CHEM;
 15 global COST_RATES_STEAM;
 16 global VALUE_HYDROGEN_FUEL VALUE_METHANE_FUEL VALUE_PROPANE_FUEL VALUE_BUTANE_FUEL;
 17 global VALUE_NATGAS_FUEL VALUE_NUM2OIL_FUEL;
 18 global ENTHALPY_PROPANE ENTHALPY_BUTANE;
 19 global MOLMASS_PROPANE MOLMASS_BUTANE;
 20 global PROFIT_S1S2_OPT;
 21 global HEAT_CAPACITY_ETHANE;
 22 global HEAT_FORMATION_ETHANE;
 23 global STEAM_30PSIA STEAM_50PSIA STEAM_100PSIA STEAM_200PSIA STEAM_500PSIA↙
STEAM_750PSIA;
 24 global HYDROGEN METHANE ETHYLENE PROPANE BUTANE;
 25 global ENTHALPY_METHANE ENTHALPY_PROPANE ENTHALPY_BUTANE HEAT_CAPACITY_ETHANE;
 26 global KT_PER_G KG_PER_KT KJ_PER_GJ MT_PER_G ENTHALPY_NAT_GAS MOLMASS_ETHANE...
 27     MOLMASS_ETHYLENE MOLMASS_NATGAS;
 28 global MT_CO2_PER_KT_METHANE MT_CO2_PER_KT_PROPANE MT_CO2_PER_KT_BUTANE ...
 29     MT_CO2_PER_KT_NATURALGAS;
 30 global TAX_CO2_PER_MT;
 31 global STEAM_PRESSURE_COL STEAM_TEMP_COL;
 32 global MOLMASS_METHANE MOLMASS_WATER BAR_PER_PSIA;
 33 global C_TO_K HEAT_CAPACITY_WATER;
 34 global R k1_f k1_r k2 k3 R_2 C_TO_K YR_PER_SEC SEC_PER_YR MOLMASS_HYDROGEN
 35 global PSA_TOGGLE ENTHALPY_HYDROGEN T_SEPARATION P_SEPARATION M3_PER_L↙
DENSITY_LIQ_WATER
 36 global MAX_CAPEX MAX_OPEX MAX_TFCI PRESS_RXTR YEARS_IN_OPERATION MILLIONBTU_PER_GJ↙
YR_PER_HR HR_PER_YR
 37 global T_OVERRIDE P_OVERRIDE STEAM_MR_OVERRIDE
 38
 39 % USER NOTES_____
 40
 41 % Note: The primary (high level) units of this script are ...
 42 % Mass          kta
 43 % Energy        GJ
 44 % Pressure      Bar
 45 % Temperature   Celcius
 46 % Moles         Moles
 47 % Value         Dollars global T_OVERRIDE P_OVERRIDE STEAM_MR_OVERRIDE
 48
 49 % [ __ ] THIS MEANS DIMENSIONLESS UNITS
 50
 51 % USER INPUTS | DESIGN PARAMETERS_____
 52
 53 % Product
 54 P_ETHYLENE_DES = 200;          % [ kta ]
 55     % Note! This design parameter's units are changed prior to the matrix def
```
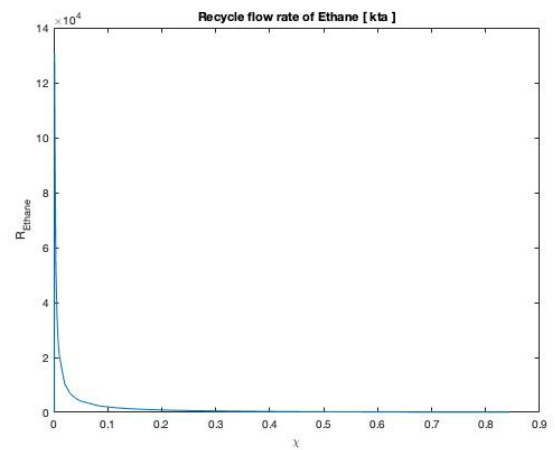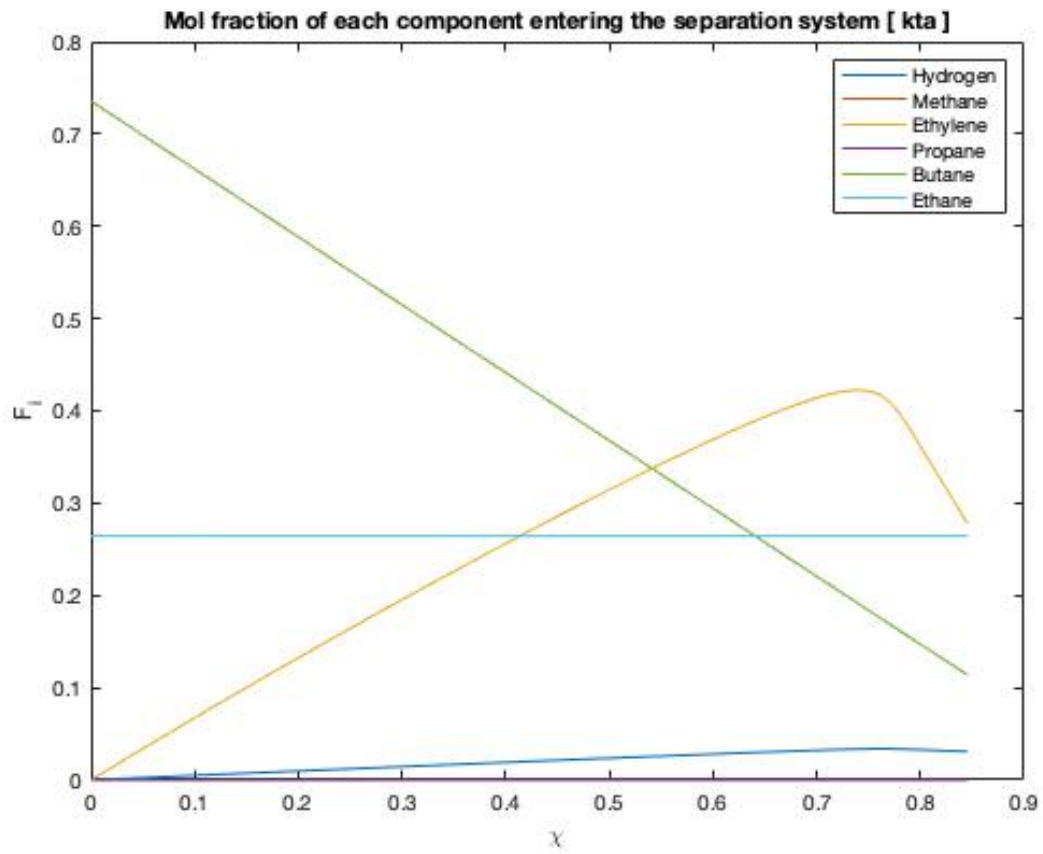
```matlab
 56
 57 YEARS_IN_OPERATION = 15 ;
 58
 59 % USER INPUTS | GLOBAL CONSTANTS_____
 60
 61 % USER INPUTS | 3D PLOT, CONTOUR, LVL 2 & 3 CALCS_____
 62
 63 % Reactor Conditions | 3D PLOT & CONTOUR PLOT (S1 S2) && THE LVL3 CALCS
 64 STEAM_TO_FEED_RATIO_MOLS = 0.6;     % [ __ ] 0.6 to 1.0
 65 TEMP_RXTR = 825;              % [ C ]
 66 PRESS_RXTR = 2;              % [ Bar ] 2 to 5 bar
 67 TEMP_ETHANE_FEED = 25;       % [ C ]
 68 CONVERSION =  0.17053;        % [ __ ] % Level 2 & 3 Calculations
 69 USERINPUT_S1 = 0.96971 ;      % [ __ ] % Level 2 & 3 Calculation  s
 70 USERINPUT_S2 = 0.00011843;     % [ __ ] % Level 2 & 3 Calculations
 71 STEAM_CHOICE = 1;
 72 %    STEAM_30PSIA = 1;
 73 %    STEAM_50PSIA = 2;
 74 %    STEAM_100PSIA = 3;
 75 %    STEAM_200PSIA = 4;
 76 %    STEAM_500PSIA = 5;
 77 %    STEAM_750PSIA = 6;
 78          % % Steam
 79          % % [ psia Temp[C] $/MT  kJ/kg ]
 80          % COST_RATES_STEAM = [
 81          %    30  121      2.38  2213;
 82          %    50  138      3.17  2159;
 83          %    100 165      4.25  2067;
 84          %    200 194      5.32  1960;
 85          %    500 242      6.74  1755;
 86          %    750 266      7.37  1634
 87          % ];
 88
 89 % Plotting | 3D PLOT & CONTOUR PLOT (S1 S2)
 90 NUM_POINTS = 10^4;
 91
 92 % USER INPUTS | RXTR TABLE PARAMETERS_____
 93
 94 % Reactor Script Parameters | RXTR TABLE OUTPUT
 95 V_MIN = 0.1;                  % [ L ]
 96 V_MAX = 4 * 10^3;               % [ L ]
 97 NUM_V_POINTS = 20;            % [ __ ]
 98
 99 P_MIN = 2;                    % [ Bar ]
100 P_MAX = 5;                    % [ Bar ]
101 NUM_P_POINTS = 2;             % [ __ ]
102
103 T_MIN = 775;                  % [ Celcius ]
104 T_MAX = 825;                  % [ Celcius ]
105 NUM_T_POINTS = 2;             % [ __ ]
106
107 STEAM_MIN = 0.6;              % [ __ ]
108 STEAM_MAX = 1.0;              % [ __ ]
109 NUM_STEAM_POINTS = 2;         % [ __ ]
110
111 % Table Overrides | RXTR TABLE OUTPUT
112 T_P_OVERRIDE = true;
113     T_P_OVERRIDE_T = true;
```

```matlab
114            T_OVERRIDE = 825;           %[C]
115      T_P_OVERRIDE_P = true;
116            P_OVERRIDE = 2;             %[Bar]
117     T_P_OVERRIDE_MR = true;
118            STEAM_MR_OVERRIDE = 0.6;%   [__]
119
120 % Output fuel costs
121 CONSOLE_OUTPUT_EFFECTIVE_VALUE_FUELS = true;
122
123 % output the cashflow matrix
124 CASHFLOW_MATRIX_OUTPUT = false;
125
126 % Output the level 2 and 3 calculations
127 OUTPUT_LVL3_FLOWRATES_TO_CONSOLE = true;
128     SANITY_CHECK_CALCULATIONS = true;
129
130 % Plot the 3D and Contour plot's
131 CALCULATE_ALL_SELECTIVITIES = true;
132     PLOT_ECON_3D = true;
133     PLOT_ECON_COUNTOUR = true;
134
135 % Output the Reactor Design tables
136 CALCULATE_REACTOR_FLOWS = true;
137
138 % PSA Toggle switch
139 PSA_TOGGLE = true;
140
141 % Do you want to add the work of the compressor to the heat flux of heating
142 % the steam from the temp it's avilable at, to the temp of the reactor?
143 ADD_COMPRESSOR_WORK_TO_STEAM_HEATFLUX = true;
144
145 % Separation System Thermodynamics
146 T_SEPARATION = 173.15;          % [ K ]
147 P_SEPARATION = PRESS_RXTR;      % [ bar ]
148 MAX_OPEX = false;        % [ __ ]
149 MAX_TFCI = false;
150 MAX_CAPEX = false;
151
152
153 % Zeolite and waste stream
154 % zeo 1.2 - 2.2 wt% absobtion = max of zeolite (g/g)
155
156 % NOTE SEARCH FOR "??" TO SEE MY ASSUMPTIONS AND OTHER NOTES IN THE CODE
157
158 % WORK OF THE COMPRESSOR HAS NOT BEEN IMPLEMENTED
159 % THE STEAM TO FEED RATIO LIKELY HAS UNIT ISSUES OF (g/g) vs (mol/mol)
160 %      I think I implemented both
161
162 %_____
163 % DON'T TOUCH ANYTHING BELOW THIS LINE
164 %_____
165
166
167 % CONSTANTS | PLOTTING_____
168
169 CONSOLE_SECTION_DIVIDER = ...
170     "_____";
171 S1_MIN = 0.01;
```

```matlab
172 S1_MAX = 1.00;
173 S1_POINTS = NUM_POINTS ^ (1/2) ;
174 S2_MIN = 0.01;
175 S2_MAX = 1.00;
176 S2_POINTS = NUM_POINTS ^ (1/2);
177 INVALID_FLOWRATE = 0;
178 Fethyl_S1S2_plotOpt = { ...
179     'S_1 Selectivity', ...
180     'S_2 Selectivity', ...
181     'Ethylene Flowrate [kta]',...
182     'P_ethylene_VS_S1_S2.jpg'};
183 PROFIT_S1S2_OPT = { ...
184     'S_1 Selectivity', ...
185     'S_2 Selectivity', ...
186     'Annual Profit [$ MM USD]',...
187     'P_ethylene_VS_S1_S2.jpg'};
188
189 % CONSTANTS | UNITS_____
190
191 % Mass
192 MT_PER_KT = 10^3;          % [ MT / kt ]
193
194 G_PER_KT = 10^9;           % [ g / kt ]
195 KT_PER_G = 10^-9;          % [ kt / g ]
196
197 KG_PER_KT = 10^6;          % [ kg / MT ]
198
199 MT_PER_G = 10^-6;          % [ MT / g ]
200
201 % Energy
202 GJ_PER_KJ = 10^-6;         % [ GJ / kJ ]
203 KJ_PER_GJ = 10^6;          % [ kJ / GJ ]
204
205 % Temperature
206 C_TO_K = 273.15;           % [ C -> K ]
207 % Value
208 MMDOLLA_PER_DOLLA = 10^-6;  % [ $ MM / $]
209 DOLLA_PER_MMDOLLA = 10^6;   % [ $ / $ MM ]
210
211 % Pressure
212 BAR_PER_PSIA = 0.0689476;   % [ Bar / Psia ]
213
214 % Time
215 YR_PER_SEC = 1 / (3.154 * 10^7);     % [ yr / s ]
216 SEC_PER_YR = 3.154 * 10^7;           % [ s / yr ]
217 YR_PER_HR = (1/8760 );               % [ yr / hr ]
218 HR_PER_YR = 8760;                    % [ hr / yr ]
219
220 % Volumes
221 M3_PER_L = 0.001;
222
223 % heat
224 MILLIONBTU_PER_GJ = 1.0551;          % [ ]
225
226 % CONSTANTS | PHYSICAL_____
227
228 DENSITY_LIQ_WATER = 10^3;            % [ kg / m^3 ]
229
```

```matlab
230 % CONSTANTS | CHEMICAL_____
231
232 % Chemical | Molar Mass
233 MOLMASS_HYDROGEN = 2.01588;              % [ g / mol ]
234     % Source :  https://webbook.nist.gov/cgi/cbook.cgi?ID=1333-74-0
235 MOLMASS_METHANE = 16.0425;               % [ g / mol ]
236     % Source :  https://webbook.nist.gov/cgi/cbook.cgi?ID=74-82-8
237 MOLMASS_WATER = 18.015;                  % [ g / mol ]
238     % source : https://pubchem.ncbi.nlm.nih.gov/compound/Water
239 MOLMASS_CO2 = 44.01;                     % [ g / mol ]
240     % Source : https://pubchem.ncbi.nlm.nih.gov/compound/Carbon-dioxide-water
241 MOLMASS_PROPANE = 44.0956;               % [ g / mol ]
242     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74986&Mask=1
243 MOLMASS_BUTANE = 58.1222;                % [ g / mol ]
244     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C106978&Mask=1
245 MOLMASS_ETHANE = 30.0690;                % [ g / mol ]
246     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74840
247 MOLMASS_ETHYLENE = 28.0532;              % [ g / mol ]
248     % Source = https://webbook.nist.gov/cgi/cbook.cgi?ID=74-85-1&Type=IR-↙
SPEC&Index=QUANT-IR,20
249 MOLMASS_NATGAS = 16.04;                  % [ g / mol ]
250     % ASSUMING NATURAL GAS IS ALL METHANE
251
252 % Chemical | Combustion Stochiometery
253 CO2_TO_METHANE_COMBUSTION_STOICH = 1;
254 CO2_TO_PROPANE_COMBUSTION_STOICH = 3;
255 CO2_TO_BUTANE_COMBUSTION_STOICH = 4;
256 C02_TO_NATGAS_COMBUSTION_STOICH = CO2_TO_METHANE_COMBUSTION_STOICH;
257     % Natural gas is asuumed to be entirely methane
258
259
260
261 % CONSTANTS | THERMODYNAMICS_____
262
263 % Gas Constant
264 R = 8.314;                               % [ J / mol K ]
265 R_2 = 0.0831446261815324;                % [ L bar / K mol ]
266
267 % Heat capacities
268 HEAT_CAPACITY_WATER = 33.79 * 10^-3;     % [ kJ / mol K ] Ref Temp = 298K
269     % Source : https://webbook.nist.gov/cgi/cbook.cgi?↙
ID=C14940637&Mask=1&Type=JANAFG&Table=on
270 HEAT_CAPACITY_ETHANE = 52.71 * 10^-3;    % [ kJ / mol K ] Reference Temp = 300K
271     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74840&Units=SI&Mask=1EFF
272
273 % Heats of Formation (at 25C)
274 HEAT_FORMATION_ETHANE = -83.8;           % [ kJ / mol ] reference Temp = std
275     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74840&Units=SI&Mask=1EFF
276 HEAT_FORMATION_METHANE = -74.87;         % [ kJ / mol ] reference Temp = std
277     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74828&Mask=1
278 HEAT_FORMATION_ETHYLENE = 52.47;         % [ kJ / mol ] reference Temp = std
279     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74851&Mask=1
280 HEAT_FORMATION_HYDROGEN = 0;             % [ kJ / mol ] reference Temp = std
281 HEAT_FORMATION_PROPANE = -104.7;         % [ kJ / mol ] reference Temp = std
282     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74986&Mask=1
283 HEAT_FORMATION_BUTANE = -125.6;          % [ kJ / mol ] reference Temp = std
284     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C106978&Mask=1
285
```

```matlab
286 % Enthalpy of combustion (std conditions)
287 ENTHALPY_HYDROGEN = 286;
288     % Source : https://chem.libretexts.org/Courses/University_of_Kentucky/UK%↙
3A_General_Chemistry/05%3A_Thermochemistry/5.3%3A_Enthalpy
289 ENTHALPY_METHANE = 890;                  % [ kJ / mol ]
290     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74828&Mask=1
291 ENTHALPY_PROPANE = 2219.2;               % [ kJ / mol ]
292     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C74986&Mask=1
293 ENTHALPY_BUTANE = 2877.5;                % [ kJ / mol ]
294     % Source : https://webbook.nist.gov/cgi/cbook.cgi?ID=C106978&Mask=1
295 ENTHALPY_NAT_GAS = ENTHALPY_METHANE;
296     % Source : https://afdc.energy.gov/fuels/natural_gas_basics.html#:~:↙
text=Natural%20gas%20is%20an%20odorless,used%20in%20the%20United%20States.
297     % Natural gas is mostly methane, so assumed to be 100% methane in the calcs
298
299 % Enthalpy of Reactions [ kJ / extent rxn]
300 ENTHALPY_RXN_1 = HEAT_FORMATION_HYDROGEN + HEAT_FORMATION_ETHYLENE ...
301                                   - HEAT_FORMATION_ETHANE;
302 ENTHALPY_RXN_2 = HEAT_FORMATION_METHANE + HEAT_FORMATION_PROPANE ...
303                                   - 2 * HEAT_FORMATION_ETHANE;
304 ENTHALPY_RXN_3 = HEAT_FORMATION_ETHANE - HEAT_FORMATION_ETHANE ...
305                                   - HEAT_FORMATION_ETHYLENE;
306 % CONSTANTS | ECONOMICS_____
307
308 %  Chemicals
309 VALUE_ETHANE = 200;          % [ $ / MT ]
310 VALUE_ETHYLENE = 900;        % [ $ / MT ]
311 VALUE_HYDROGEN_CHEM = 1400;  % [ $ / MT ]
312
313 % Steam
314 % [ psia Temp[C] $/MT  kJ/kg ]
315 COST_RATES_STEAM = [
316     30  121     2.38  2213;
317     50  138     3.17  2159;
318     100 165     4.25  2067;
319     200 194     5.32  1960;
320     500 242     6.74  1755;
321     750 266     7.37  1634
322 ];
323
324 % Accessing the Steam P,T Data
325     STEAM_PRESSURE_COL = 2;
326     STEAM_TEMP_COL = 1;
327     STEAM_COST_COL = 3;
328     STEAM_30PSIA = 1;
329     STEAM_50PSIA = 2;
330     STEAM_100PSIA = 3;
331     STEAM_200PSIA = 4;
332     STEAM_500PSIA = 5;
333     STEAM_750PSIA = 6;
334
335 % Economic | Fuel
336 VALUE_HYDROGEN_FUEL = 3;         % [ $ / GJ ]
337 VALUE_METHANE_FUEL = 3;          % [ $ / GJ ]
338 VALUE_PROPANE_FUEL = 3;          % [ $ / GJ ]
339 VALUE_BUTANE_FUEL = 3;           % [ $ / GJ ]
340 VALUE_NATGAS_FUEL = 3;           % [ $ / GJ ]
341 VALUE_NUM2OIL_FUEL = 4.5;        % [ $ / US Gallon ]
```

```matlab
342
343 % Economics | Enviormental
344 TAX_CO2_PER_MT = 125;                % [ $ / MT ]
345
346 % [$ / GJ]  = 1GJ(basis) * (KJ / GJ)   * (mol gas / KJ) *         (mol CO2 / mol↙
gas)         *  (g / mol C02)*(MT / g) * ($ / MT)
347 TAX_CO2_PER_GJ_METHANE = KJ_PER_GJ * (1 / ENTHALPY_METHANE) *↙
CO2_TO_METHANE_COMBUSTION_STOICH * MOLMASS_CO2 * MT_PER_G * TAX_CO2_PER_MT;
348 TAX_CO2_PER_GJ_PROPANE = KJ_PER_GJ * (1 / ENTHALPY_PROPANE) *↙
CO2_TO_PROPANE_COMBUSTION_STOICH * MOLMASS_CO2 * MT_PER_G * TAX_CO2_PER_MT;
349 TAX_CO2_PER_GJ_BUTANE = KJ_PER_GJ * (1 / ENTHALPY_BUTANE) *↙
CO2_TO_BUTANE_COMBUSTION_STOICH * MOLMASS_CO2 * MT_PER_G * TAX_CO2_PER_MT;
350 TAX_CO2_PER_GJ_NATGAS = TAX_CO2_PER_GJ_METHANE; %
351
352 % Chemistry | MT of C02 per KT of Fuel used
353 % (MT CO2) = 1KT(basis) * (g / KT) * (mol gas/ g gas) *
354 MT_CO2_PER_KT_METHANE = G_PER_KT * (1/MOLMASS_METHANE) *...
355     ... % (mol CO2 / mol gas) *         (g CO2 / mol CO2) * (MT / g)
356     CO2_TO_METHANE_COMBUSTION_STOICH * MOLMASS_CO2 * MT_PER_G;
357 MT_CO2_PER_KT_PROPANE = G_PER_KT * (1/MOLMASS_PROPANE) *...
358     CO2_TO_PROPANE_COMBUSTION_STOICH * MOLMASS_CO2 * MT_PER_G;
359 MT_CO2_PER_KT_BUTANE = G_PER_KT * (1/MOLMASS_BUTANE) *...
360     CO2_TO_BUTANE_COMBUSTION_STOICH * MOLMASS_CO2 * MT_PER_G;
361 MT_CO2_PER_KT_NATURALGAS = MT_CO2_PER_KT_METHANE;
362
363 % FUNCTIONS | FLOWRATE_____
364
365 P_ETHYLENE = P_ETHYLENE_DES;
366 P_ETHYLENE_DES = P_ETHYLENE_DES * (1 / MOLMASS_ETHYLENE);
367 P_PROPANE = @(s1, s2)      (s2 / s1 *P_ETHYLENE_DES) * ...
368                               MOLMASS_PROPANE;
369 P_BUTANE = @(s1, s2)      (P_ETHYLENE_DES*(1/(2*s1) - s2/s1 - 1/2)) * ...
370                               MOLMASS_BUTANE;
371 F_ETHANE = @(s1, s2)      (P_ETHYLENE_DES / s1) * ...
372                               MOLMASS_ETHANE;
373 P_METHANE = @(s1, s2) (s2 / s1 * P_ETHYLENE_DES) * ...
374                               MOLMASS_METHANE;
375 P_HYDROGEN = @(s1, s2) (P_ETHYLENE_DES * ((1/(2*s1) - s2/s1 + 1/2))) * ...
376                               MOLMASS_HYDROGEN;
377
378 % FUNCTIONS | EXTENT OF REACTION_____
379
380 % Returns molar flowrates [ mol / yr ]
381 get_xi = @(flowrates) [ flowrates(HYDROGEN) * G_PER_KT / MOLMASS_HYDROGEN, ...
382                     flowrates(PROPANE) * G_PER_KT / MOLMASS_PROPANE, ...
383                     flowrates(BUTANE) * G_PER_KT / MOLMASS_BUTANE ];
384
385 % FUNCTIONS | VALIDATION_____
386
387 flowrates_valid = @( flowrates ) all(flowrates >= 0);
388
389 % FUNCTIONS | ECONOMICS_____
390
391 % ($ / yr) =                  (kta) *   (MT / KT) * ($ / MT)
392 value_ethane = @(P_ethane) P_ethane * MT_PER_KT * VALUE_ETHANE;
393 value_ethylene = @(P_ethylene) P_ethylene * MT_PER_KT * VALUE_ETHYLENE;
394 value_h2_chem = @(P_h2_chem) P_h2_chem * MT_PER_KT * VALUE_HYDROGEN_CHEM;
395 value_methane = @(P_methane) P_methane * MT_PER_KT * VALUE_METHANE_FUEL;
```

```matlab
396 value_propane = @(P_propane) P_propane * MT_PER_KT * VALUE_PROPANE_FUEL;
397 value_butane = @(P_butane) P_butane * MT_PER_KT * VALUE_BUTANE_FUEL;
398
399 % ($ / yr) =                             (kta) *  (MT / kt) * ($ / MT)
400 cost_steam = @(F_steam, steam_rate) F_steam * MT_PER_KT * steam_rate;
401
402 % FUNCTIONS | THEROMODYNAMICS_____
403 % (GJ / yr) =                          (kta) *  (g / KT)   * (mol gas/ g gas)   *↙
(kJ / mol K)          * (GJ / KJ) * (K)
404 heat_ethane = @(F_ethane, T0, Tf) F_ethane * G_PER_KT * (1 / MOLMASS_ETHANE) *↙
HEAT_CAPACITY_ETHANE * GJ_PER_KJ * (Tf - T0);
405
406 % (GJ / yr)  =      (mol / yr) * (kJ / mol) *   (GJ / kJ)
407 heat_rxn1 = @(xi_1) xi_1 * ENTHALPY_RXN_1 * GJ_PER_KJ;
408 heat_rxn2 = @(xi_2) xi_2 * ENTHALPY_RXN_2 * GJ_PER_KJ;
409 heat_rxn3 = @(xi_3) xi_3 * ENTHALPY_RXN_3 * GJ_PER_KJ;
410 heat_rxn = @(xi) heat_rxn1(xi(1)) + heat_rxn2(xi(2)) + heat_rxn3(xi(3));
411
412 % FUNCTIONS | RATE CONTANTS_____
413
414 % T is [ Kelvin ]  R is [ J / mol K ]
415 k1_f = @(T) (4.652 * 10^13) * exp( (-273000 / (R * (T ))));
416 k1_r = @(T) (9.91 * 10^8) * exp( (-137800 / (R * (T ))));
417 k2 = @(T) (4.652 * 10^11) * exp( (-273000 / (R * (T ))));
418 k3 = @(T) (7.083 * 10^13) * exp( (-252600 / (R * (T ))));
419
420
421 % DESIGN PARAMS_____
422 STEAM_TO_FEED_RATIO_MASS = (MOLMASS_WATER / MOLMASS_ETHANE) *↙
STEAM_TO_FEED_RATIO_MOLS;
423
424
425 % SCRIPT_____
426
427 % Economics | Post-Tax Value of different fuel sources
428 if (CONSOLE_OUTPUT_EFFECTIVE_VALUE_FUELS)
429     disp(" [ $ / GJ ] ")
430     EFFECTIVE_VALUE_HYDROGEN_FUEL = VALUE_HYDROGEN_FUEL
431     EFFECTIVE_VALUE_METHANE_FUEL = VALUE_METHANE_FUEL + TAX_CO2_PER_GJ_METHANE
432     EFFECTIVE_VALUE_PROPANE_FUEL = VALUE_PROPANE_FUEL + TAX_CO2_PER_GJ_PROPANE
433     EFFECTIVE_VALUE_BUTANE_FUEL = VALUE_BUTANE_FUEL + TAX_CO2_PER_GJ_BUTANE
434     EFFECTIVE_VALUE_NAT_GAS_FUEL = VALUE_NATGAS_FUEL + TAX_CO2_PER_GJ_NATGAS
435 %   EFFECTIVE_VALUE_NUM2_FUEL = VALUE_NATGAS_FUEL + TAX_CO2_PER_GJ_NUM2;
436
437 end
438
439 if (OUTPUT_LVL3_FLOWRATES_TO_CONSOLE)
440
441     % Calculate the flow rates of each species (kta)
442     P_hydrogen = P_HYDROGEN(USERINPUT_S1, USERINPUT_S2);
443     P_methane = P_METHANE(USERINPUT_S1, USERINPUT_S2);
444     P_ethylene = P_ETHYLENE;
445     P_propane = P_PROPANE(USERINPUT_S1, USERINPUT_S2);
446     P_butane = P_BUTANE(USERINPUT_S1, USERINPUT_S2);
447     F_ethane = F_ETHANE(USERINPUT_S1, USERINPUT_S2);
448     P_flowrates = [ P_hydrogen, P_methane, P_ethylene, P_propane, P_butane ];
449
450     disp(CONSOLE_SECTION_DIVIDER)
```

```matlab
451        if (flowrates_valid(P_flowrates))
452
453            fprintf("Flowrates for the reactor given that s1 = %f, s2 = %f conv = %↙
f\n\n", ...
454                USERINPUT_S1, USERINPUT_S2, CONVERSION)
455
456            disp(CONSOLE_SECTION_DIVIDER)
457            disp("Level 2 Flowrates  in / out of the entire plant [ kt / yr ]")
458            P_hydrogen
459            P_methane
460            P_ethylene
461            P_propane
462            P_butane
463
464            disp("Fresh Feed Flowrate")
465            F_ethane
466
467            disp(CONSOLE_SECTION_DIVIDER)
468            disp("Level 3 Flowrates [ kt / yr ] ")
469
470            disp("Recycle Stream Flowrate")
471
472            R_ethane = F_ethane * ((1-CONVERSION) / (CONVERSION))
473            % R_ethane = (P_ethylene/USERINPUT_S1) * ((1-CONVERSION)/CONVERSION)
474
475            disp("Reactor Flowrates")
476
477            F_ethane_into_reactor = R_ethane + F_ethane
478
479            if SANITY_CHECK_CALCULATIONS
480                disp(CONSOLE_SECTION_DIVIDER)
481                disp("Sanity Checking the Calculations")
482                Conservation_of_mass = F_ethane - sum(P_flowrates)
483                if Conservation_of_mass
484                    fprintf("WARNING : YOU ARE NOT CONSERVING MASS\n\n")
485                end
486            end
487        else
488            disp("ERROR : Selectivities S1 S2 chosen are not physically possible")
489        end
490 end
491
492 % SCRIPT | PLOTTING_____
493
494 if (CALCULATE_ALL_SELECTIVITIES)
495     disp(CONSOLE_SECTION_DIVIDER)
496     disp("Calculating all selectivities... ")
497     % Iterates through each value of selectivities S1 and S2 to find the economic
498     % potential for different reaction conditions
499     s1_domain = linspace(S1_MIN, S1_MAX, S1_POINTS);
500     s2_domain = linspace(S2_MIN, S2_MAX, S2_POINTS);
501     [s1_mesh, s2_mesh] = meshgrid(s1_domain, s2_domain);
502     % All flowrates are initialized as matricies of zeros
503     ethylene_flowrates = (s1_mesh + s2_mesh) .* 0;
504     hydrogen_flowrates = (s1_mesh + s2_mesh) .* 0;
505     methane_flowrates = (s1_mesh + s2_mesh) .* 0;
506     ethylene_flowrates = (s1_mesh + s2_mesh) .* 0;
507     propane_flowrates = (s1_mesh + s2_mesh) .* 0;
```

```matlab
508        butane_flowrates = (s1_mesh + s2_mesh) .* 0;
509        ethane_flowrates = (s1_mesh + s2_mesh) .* 0;
510
511        profit = (s1_mesh + s2_mesh) .* 0;
512
513        % Flow rate Indicies | For the flowrates(i) array
514        HYDROGEN = 1;
515        METHANE = 2;
516        ETHYLENE = 3;
517        PROPANE = 4;
518        BUTANE = 5;
519
520        i = 1;
521        for s1 = s1_domain
522            for s2 = s2_domain
523
524                P_hydrogen = P_HYDROGEN(s1, s2);
525                P_methane = P_METHANE(s1, s2);
526                P_ethylene = P_ETHYLENE;
527                P_propane = P_PROPANE(s1, s2);
528                P_butane = P_BUTANE(s1, s2);
529                F_ethane = F_ETHANE(s1, s2);
530
531                P_flowrates = [ P_hydrogen, P_methane, P_ethylene, P_propane, P_butane↙
];
532
533                if (flowrates_valid(P_flowrates))
534
535                    % Store for plotting (kta)
536                    hydrogen_flowrates(i) = P_HYDROGEN(s1, s2);
537                    methane_flowrates(i) = P_METHANE(s1, s2);
538                    ethylene_flowrates(i) = P_ETHYLENE;
539                    propane_flowrates(i) = P_PROPANE(s1, s2);
540                    butane_flowrates(i) = P_BUTANE(s1, s2);
541                    ethane_flowrates(i) = F_ETHANE(s1, s2);
542
543                    % F_ethane = F_ETHANE(select_1(i), select_2(i));
544                    % F_fresh_ethane = F_ethane;
545                    % F_ethane_rxtr = F_ethane(i) * ( conversion(i) / (1 - conversion↙
(i)) );
546
547                    xi = [];
548                    % Calculate the heat flux needed to keep reactor isothermal
549                    heat_flux = 0;
550                    xi = get_xi(P_flowrates);
551                    F_steam = STEAM_TO_FEED_RATIO_MASS * F_ethane;
552                    heat_flux = heat_flux + heat_ethane(F_ethane, TEMP_ETHANE_FEED,↙
TEMP_RXTR);
553                    % heat_flux = heat_flux + heat_ethane(F_ethane_into_reactor,↙
TEMP_SEPARATION, TEMP_RXTR);
554                    heat_flux = heat_flux + heat_steam(F_steam, STEAM_CHOICE,↙
PRESS_RXTR, TEMP_RXTR) ;
555                    heat_flux = heat_flux + heat_rxn(xi);
556
557        %        % Use the heat flux to calculate the fuel cost
558                    [combusted_fuel_flow_rates, heat_flux_remaining] = fuel_combustion↙
(heat_flux, P_flowrates);
559
```

```matlab
560                    % Calculate how much natural gas you needed to combust
561                    F_natural_gas = natgas_combustion(heat_flux_remaining);
562
563                    % Determine how much of the product streams were combusted to keep↙
the reactor isothermal
564
565                    combusted_hydrogen = combusted_fuel_flow_rates(HYDROGEN);
566                    combusted_methane = combusted_fuel_flow_rates(METHANE);
567                    combusted_propane = combusted_fuel_flow_rates(PROPANE);
568                    combusted_butane = combusted_fuel_flow_rates(BUTANE);
569
570     %             % VALUE CREATED | Primary Products
571                    profit(i) = profit(i) + value_ethylene(P_ethylene);
572                    profit(i) = profit(i) + value_h2_chem(P_hydrogen -↙
combusted_hydrogen);
573
574                    % VALUE CREATED | Non-combusted fuels
575                    % profit(i) = profit(i) + value_methane(P_methane -↙
combusted_methane);
576                        % ?? I don't think you can sell methane. IH - need to
577                        % determine energy requirements for compressors +
578                        % separation + cooling (will likely need to purchase
579                        % Nat Gas)
580                    profit(i) = profit(i) + value_propane(P_propane -↙
combusted_propane);
581                    profit(i) = profit(i) + value_butane(P_butane - combusted_butane);
582
583                    % COSTS INCURRED
584                    profit(i) = profit(i) - tax_C02(combusted_fuel_flow_rates,↙
F_natural_gas);
585                    profit(i) = profit(i) - cost_steam(F_steam, COST_RATES_STEAM↙
(STEAM_CHOICE, STEAM_COST_COL));
586                    profit(i) = profit(i) - value_ethane(F_ethane);
587                    profit(i) = profit(i) - cost_natural_gas_fuel(F_natural_gas);
588                    profit(i) = profit(i) - cost_waste_stream(F_steam);
589
590                    % profit(i) = profit(i) - cost
591
592
593                else
594                    profit(i) = INVALID_FLOWRATE;
595                    ethylene_flowrates(i) = INVALID_FLOWRATE;
596                end
597                i = i + 1;
598            end
599      end
600
601      profit = profit ./ 10^6; % Convert to Millions of dollars
602      profit(profit < 0) = 0; % remove irrelvant data
603
604      if (PLOT_ECON_COUNTOUR)
605          disp("Plotting EP Contour Map")
606          plot_contour(s1_mesh, s2_mesh, profit, PROFIT_S1S2_OPT);
607      end
608      if (PLOT_ECON_3D)
609          disp("Plotting 3D EP Surface Function")
610          plot_3D(s1_mesh, s2_mesh, profit, PROFIT_S1S2_OPT);
611      end
```

```matlab
612
613      % Prepare the array of flow rate matrices
614      % flowRatesArray = {hydrogen_flowrates, methane_flowrates, ethylene_flowrates,↙
propane_flowrates, butane_flowrates, ethane_flowrates};
615
616      % Call the function with the desired row
617      % plotFlowRatesForRow(4, flowRatesArray); % To plot the first row across all↙
matrices
618 end
619
620
621 % SCRIPT | REACTOR _____
622
623 T_RANGE = linspace(T_MIN, T_MAX, NUM_T_POINTS);
624 P_RANGE = linspace(P_MIN, P_MAX, NUM_P_POINTS);
625 STEAM_RANGE = linspace(STEAM_MIN, STEAM_MAX, NUM_STEAM_POINTS);
626 V_RANGE = [V_MIN, V_MAX]; % WARNING THESE ARE IN LITERS
627 % H2 Methane Ethane Propane Butane Ethylene
628 F_INTIAL_COND = [ 0; 0; 0; 0; 0; 10]; % These are in kta
629
630      % Product flow rate indicies
631      HYDROGEN = 1;
632      METHANE = 2;
633      ETHYLENE = 3;
634      PROPANE = 4;
635      BUTANE = 5;
636
637      % Feed flow rate index
638      ETHANE = 6;
639 % npv_T_P_MR = zeros(length(T_RANGE), length(P_RANGE), length(STEAM_RANGE), 1);
640 npv_T_P_MR = cell(length(T_RANGE), length(P_RANGE), length(STEAM_RANGE) );
641
642 i = 1;
643 j = 1;
644 k = 1;
645 if (CALCULATE_REACTOR_FLOWS)
646     disp("Reactor Script ")
647     for T_i = T_RANGE
648         for P_i = P_RANGE
649             for MR_S_i = STEAM_RANGE
650
651                 % override the T_i and P_i with user input
652                 if T_P_OVERRIDE
653                     disp("WARNING: OVERRIDE HAS BEEN ACTIVATED")
654                     if T_P_OVERRIDE_T
655                         T_i = T_OVERRIDE;
656                     end
657                     if T_P_OVERRIDE_P
658                         P_i = P_OVERRIDE;
659                     end
660                     if T_P_OVERRIDE_MR
661                         MR_S_i = STEAM_MR_OVERRIDE;
662                     end
663                 end
664
665                 fprintf("\n\nT = %f [C], P = %f [bar] MR = %f [__]\n", T_i, P_i,↙
MR_S_i)
666
```

```
667                    % Setup the PFR Design Equations
668
669                    % BASIS↵
CALCULATIONS_____
670
671                    % CONVERT TO↵
MOLES_____
672                    % Convert all of the initial conditions to mol / s
673                    % (mol / s) =        (kt / yr) *           (g / kt) *   ( mol↵
/ g )        * ( yr / s)
674                    F_INTIAL_COND(METHANE) = F_INTIAL_COND(METHANE) * G_PER_KT *↵
(1/MOLMASS_METHANE) * YR_PER_SEC;
675                    F_INTIAL_COND(HYDROGEN) = F_INTIAL_COND(HYDROGEN) * G_PER_KT *↵
(1/MOLMASS_HYDROGEN) * YR_PER_SEC;
676                    F_INTIAL_COND(ETHANE) = F_INTIAL_COND(ETHANE) * G_PER_KT *↵
(1/MOLMASS_ETHANE) * YR_PER_SEC;
677                    F_INTIAL_COND(ETHYLENE) = F_INTIAL_COND(ETHYLENE) * G_PER_KT *↵
(1/MOLMASS_ETHYLENE) * YR_PER_SEC;
678                    F_INTIAL_COND(PROPANE) = F_INTIAL_COND(PROPANE) * G_PER_KT *↵
(1/MOLMASS_PROPANE) * YR_PER_SEC;
679
680                    % Calculate the molar flow rate of the steam
681                    % mol/s = __    * mol / s
682                    F_steam = MR_S_i * F_INTIAL_COND(ETHANE);
683
684                    % Solve the system ODE's
685                    %   (L, mol / s)          (L, mol/s, Celcius, Bar, mol/s)
686                    odes = @(V, F) reactionODEs(V, F, T_i, P_i, F_steam);
687                    [V_soln_ODE, F_soln_ODE] = ode45(odes, V_RANGE, F_INTIAL_COND);
688
689                    % Calculate the conversion
690                    conversion = (F_INTIAL_COND(ETHANE) – F_soln_ODE(:, ETHANE)) /↵
F_INTIAL_COND(ETHANE);
691
692                    % put handles length of the solution and the initial ethane flow
693                    len = length(F_soln_ODE(:, 1));
694                    F_ethane_initial = ones(len, 1) * F_INTIAL_COND(ETHANE);
695
696                    % Calculate the Selectivities, for each row (aka V_rxtr)
697                    select_1 = (F_soln_ODE(:, ETHYLENE) ) ./ (F_ethane_initial –↵
F_soln_ODE(:, ETHANE));
698                    select_2 = (F_soln_ODE(:, PROPANE) ) ./ (F_ethane_initial –↵
F_soln_ODE(:, ETHANE));
699
700                    % Calculate the inlet volumetric flow rate
701                    % (L / s) ????????????????
702                    P_sum = F_soln_ODE(:, HYDROGEN:BUTANE);
703                    % Turn these constants into vectors to operation is valid
704                    F_steam = ones(length(P_sum(:,1)), 1) .* F_steam;
705                    % put handles on terms, to make the code readable
706                    sum_flowrates_into_reactor = F_INTIAL_COND(ETHANE) + F_steam;
707                    % Calculate the flow rate into the reactor
708                    q0 = (R_2  * (T_i + C_TO_K) / P_i) .* sum_flowrates_into_reactor;
709                        % This is F.30 in the 'Design PFR Algorithm Appendix'
710
711                    % PLANT↵
CALCULATIONS_____
712
```

```
713                    % Calculate the the flowrates of the plant sized reactor given S1,↵
S2 from ODE's
714                    F_ethane = [];
715                    P_ethylene = [];
716                    for row = 1:length(select_1)
717                        % mol / s        = (kt / yr)   * (g / kt)  * (mol / g)↵
* (yr / s)
718                        P_ethylene(row, 1) = P_ETHYLENE .* G_PER_KT .*↵
(1/MOLMASS_ETHYLENE) * YR_PER_SEC;
719                    end
720
721                    % Calculate the scaling factor of the plant, from the basis
722                    % mol / mol = ...
723                    scaling_factor = P_ethylene(:, 1) ./ F_soln_ODE(:, ETHYLENE);
724
725                    % Calculate the volume of the plant sized reactor
726                    % L / s = ( L / s )        * (    (mol / s ) ) / (    (mol / s)↵
)
727                    %         BASIS           *     PLANT_FLOW   /      BASIS_FLOW
728                    V_plant = V_soln_ODE(:, 1) .* scaling_factor;
729
730                    % cost of the reactor
731                    cost_rxt_vec = zeros(size(V_plant));
732                    for row = 1:length(V_plant)
733                        % ( $ )
734                        cost_rxt_vec(row) = cost_reactor(V_plant(row,1) * M3_PER_L);
735                        cost_rxt_vec(row) = cost_rxt_vec(row) / YEARS_IN_OPERATION;
736                    end
737
738                    % inlet flow of the plant scaled reactor
739                    q0_plant = q0(:, 1) .* scaling_factor;
740                        % Eqn F.35 in 'Design PFR Algorithm Appendix'
741
742                    % Scaling all of the molar flowrates to the size of the plant
743                    F_soln_ODE(:, METHANE) = F_soln_ODE(:, METHANE) .* scaling_factor;
744                    F_soln_ODE(:, HYDROGEN) = F_soln_ODE(:, HYDROGEN) .* scaling_factor;
745                    F_soln_ODE(:, ETHANE) = F_soln_ODE(:, ETHANE) .* scaling_factor;
746                    F_soln_ODE(:, ETHYLENE) = F_soln_ODE(:, ETHYLENE) .* scaling_factor;
747                    F_soln_ODE(:, BUTANE) = F_soln_ODE(:, BUTANE) .* scaling_factor;
748                    F_soln_ODE(:, PROPANE) = F_soln_ODE(:, PROPANE) .* scaling_factor;
749
750                    % CONVERT BACK TO↵
MASS_____
751
752                    % convert back to kta
753                    % kt / yr =  mol / s   * g / mol        * kt / g   * s / yr
754                    F_soln_ODE(:, METHANE) = F_soln_ODE(: ,METHANE) * MOLMASS_METHANE *↵
KT_PER_G * SEC_PER_YR;
755                    F_soln_ODE(:, ETHANE) = F_soln_ODE(:, ETHANE) * MOLMASS_ETHANE *↵
KT_PER_G * SEC_PER_YR;
756                    F_soln_ODE(:, HYDROGEN) = F_soln_ODE(:, HYDROGEN) * MOLMASS_HYDROGEN↵
* KT_PER_G * SEC_PER_YR;
757                    F_soln_ODE(:, ETHYLENE) = F_soln_ODE(:, ETHYLENE) * MOLMASS_ETHYLENE↵
* KT_PER_G * SEC_PER_YR;
758                    F_soln_ODE(:, BUTANE) = F_soln_ODE(:, BUTANE) * MOLMASS_BUTANE *↵
KT_PER_G * SEC_PER_YR;
759                    F_soln_ODE(:, PROPANE) = F_soln_ODE(:, PROPANE) * MOLMASS_PROPANE *↵
KT_PER_G * SEC_PER_YR;
```

```matlab
760
761                    % Check if you're conserving mass
762                    conserv_mass = zeros(length(F_soln_ODE(:,1)), 1);
763                    npv = zeros(length(F_soln_ODE(:,1)), 1);
764                    fxns.separationCosts = zeros(length(F_soln_ODE(:,1)), 1);
765                    fxns.furnaceCosts = zeros(length(F_soln_ODE(:,1)), 1);
766                    fxns.F_steam = zeros(length(F_soln_ODE(:,1)), 1);
767                    fxns.F_fresh_ethane = zeros(length(F_soln_ODE(:,1)), 1);
768                    xi = [ 0 , 0, 0];   %init
769
770                    % ECONOMIC↵
CALCULATIONS_____
771                    profit = zeros(length(F_soln_ODE(:,1)), 1);
772                    for i = 1:length(F_soln_ODE(:, 1))
773
774                        % DEBUGGING
775                        if i > 500
776                            disp("")
777                        end
778                        % P_flowrates = [ P_hydrogen, P_methane, P_ethylene, P_propane,↵
P_butane ];
779                        P_flowrates = F_soln_ODE(i , HYDROGEN:BUTANE);
780
781                        P_hydrogen = P_flowrates(HYDROGEN);
782                        P_methane = P_flowrates(METHANE);
783                        P_ethylene = P_flowrates(ETHYLENE);
784                        P_propane = P_flowrates(PROPANE);
785                        P_butane = P_flowrates(BUTANE);
786
787                        F_fresh_ethane = F_ETHANE(select_1(i), select_2(i));
788                        R_ethane = F_fresh_ethane * ( ( 1 – conversion(i)) / conversion↵
(i) );
789                        R_ethane = F_soln_ODE(i, ETHANE);
790                            % ?? These two values R should be the same
791
792                        if (~flowrates_valid(P_flowrates))
793                            disp("WARNING SOME FLOWATES MAY BE INVALID")
794                        end
795
796                        % Calculate the heat flux needed to keep reactor isothermal
797                        heat_flux = 0;
798                        xi = get_xi(P_flowrates);
799                        F_steam = STEAM_TO_FEED_RATIO_MASS * (F_fresh_ethane +↵
R_ethane);
800                        heat_flux = heat_flux + heat_ethane(F_fresh_ethane,↵
TEMP_ETHANE_FEED, TEMP_RXTR);
801                        heat_flux = heat_flux + heat_ethane(R_ethane, T_SEPARATION –↵
C_TO_K, TEMP_RXTR);
802                        heat_flux = heat_flux + heat_steam(F_steam, STEAM_CHOICE,↵
PRESS_RXTR, TEMP_RXTR) ;
803                        heat_flux = heat_flux + heat_rxn(xi);
804
805                        % Use the heat flux to calculate the fuel cost
806                        [combusted_fuel_flow_rates, heat_flux_remaining] =↵
fuel_combustion(heat_flux, P_flowrates);
807
808                        % Calculate how much natural gas you needed to combust
809                        F_natural_gas = natgas_combustion(heat_flux_remaining);
```

```matlab
810
811                          % Determine how much of the product streams were combusted to↙
keep the reactor isothermal
812                             combusted_hydrogen = combusted_fuel_flow_rates(HYDROGEN);
813                             combusted_methane = combusted_fuel_flow_rates(METHANE);
814                             combusted_propane = combusted_fuel_flow_rates(PROPANE);
815                             combusted_butane = combusted_fuel_flow_rates(BUTANE);
816
817                          % VALUE CREATED | Primary Products
818                          profit(i, 1) = profit(i, 1) + value_ethylene(P_ethylene);
819                          profit(i, 1) = profit(i, 1) + value_h2_chem(P_hydrogen -↙
combusted_hydrogen);
820
821                          % VALUE CREATED | Non-combusted fuels
822                          % The commented line can be removed or modified as per the↙
context.
823                          % profit(i, 1) = profit(i, 1) + value_methane(P_methane -↙
combusted_methane);
824                          profit(i, 1) = profit(i, 1) + value_propane(P_propane -↙
combusted_propane);
825                          profit(i, 1) = profit(i, 1) + value_butane(P_butane -↙
combusted_butane);
826
827                          % COSTS INCURRED
828                          profit(i, 1) = profit(i, 1) - tax_C02(combusted_fuel_flow_rates,↙
F_natural_gas);
829                          profit(i, 1) = profit(i, 1) - cost_steam(F_steam,↙
COST_RATES_STEAM(STEAM_CHOICE, STEAM_COST_COL));
830                          profit(i, 1) = profit(i, 1) - value_ethane(F_fresh_ethane);
831                          profit(i, 1) = profit(i, 1) - cost_natural_gas_fuel↙
(F_natural_gas);
832                          profit(i, 1) = profit(i, 1) - cost_waste_stream(F_steam);
833                          profit(i, 1) = profit(i, 1) - cost_separation_system↙
(P_flowrates, F_steam, R_ethane);
834                          profit(i, 1) = profit(i, 1) - calculate_installed_cost↙
(heat_flux);
835
836                          % Store Data For analysis
837                          fxns.separationCosts(i, 1) = cost_separation_system(P_flowrates,↙
F_steam, R_ethane);
838                          fxns.furnaceCosts(i, 1)  = calculate_installed_cost(heat_flux);
839                          fxns.F_steam(i, 1) = F_steam;
840                          fxns.F_fresh_ethane(i, 1) = F_fresh_ethane;
841
842                          % Checking if I still have any sanity left after this, who↙
knows...
843                          conserv_mass(i, 1) = F_fresh_ethane - sum(P_flowrates);
844
845                          % NPV params
846                          npv_params.mainProductRevenue = value_ethylene(P_ethylene) *↙
MMDOLLA_PER_DOLLA;
847                          npv_params.byProductRevenue = value_h2_chem(P_hydrogen -↙
combusted_hydrogen) * MMDOLLA_PER_DOLLA;
848                          npv_params.rawMaterialsCost = value_ethane(F_fresh_ethane) *↙
MMDOLLA_PER_DOLLA;
849                          npv_params.utilitiesCost = cost_steam(F_steam, COST_RATES_STEAM↙
(STEAM_CHOICE, STEAM_COST_COL)) * MMDOLLA_PER_DOLLA;
850                          npv_params.CO2sustainabilityCharge = tax_C02↙
```

```matlab
(combusted_fuel_flow_rates, F_natural_gas) * MMDOLLA_PER_DOLLA;
851                         npv_params.conversion = conversion(i);
852                         % npv_params.ISBLcapitalCost = (cost_rxt_vec(i) +↵
cost_separation_system(P_flowrates, F_steam, R_ethane)) * MMDOLLA_PER_DOLLA;
853                         npv_params.ISBLcapitalCost = (cost_rxt_vec(i) + ...
854                                     cost_separation_system(P_flowrates,↵
F_steam, R_ethane) + ...
855                                     calculate_installed_cost(heat_flux)) *↵
MMDOLLA_PER_DOLLA;
856
857                         % NPV calculations
858                         cf = get_npv(npv_params);
859                         npv(i, 1) = cf.lifetime_npv;
860                         if conversion(i) > 0.67 && conversion(i) < 0.70
861                             cf = get_npv(npv_params);
862                             ideal_cf = cf;
863                             ideal_params = npv_params;
864                             ideal_conversion = conversion(i);
865                             ideal_lifetimeNpv = cf.lifetime_npv;
866                         end
867
868                 end
869
870                 % Assuming A is your matrix
871                 % A = [1 2 3; 4 5 6; 7 8 9; 10 11 12]; % Example matrix
872
873                 % Find the maximum value in the 3rd column and its row index
874                 % [maxValue, rowIndex] = max(A(:,3));
875
876                 % [maxValue, maxRowIndex] = max(npv(:,1));
877
878                 % max value NPV for all T P MR
879                 % npv_T_P_MR(i,j,k) = npv(maxRowIndex, 1);
880                 % npv_T_P_MR(i,j,k) = npv(:,1);
881 %               temp  = npv);
882 %               npv_T_P_MR{i,j,k} = npv;
883
884
885                 % % Plotting the Capstone plots
886                 % fxns.conversion = conversion;
887                 % fxns.V_plant = V_plant;
888                 % fxns.select_1 = select_1;
889                 % fxns.select_2 = select_2;
890                 % fxns.npv = npv;
891                 % fxns.recycle = F_soln_ODE( : , ETHANE);
892                 % fxns.freshFeedRawMaterials = fxns.F_fresh_ethane + fxns.F_steam;
893                 % fxns.productionRateRxnProducts = F_soln_ODE( : , HYDROGEN :↵
BUTANE);
894                 % fxns.F_rxtr_in_total = fxns.F_fresh_ethane + fxns.recycle + fxns.↵
F_steam;
895                 % fxns.F_sep = sum(F_soln_ODE(: , HYDROGEN : ETHANE), 2) + fxns.↵
F_steam;
896                 % fxns.x_hydrogen_sep = F_soln_ODE( : , HYDROGEN) ./ fxns.F_sep;
897                 % fxns.x_methane_sep = F_soln_ODE( : , METHANE) ./ fxns.F_sep;
898                 % fxns.x_ethylene = F_soln_ODE( : , ETHYLENE) ./ fxns.F_sep;
899                 % fxns.x_propane_sep = F_soln_ODE( : , PROPANE) ./ fxns.F_sep;
900                 % fxns.x_butane_sep = F_soln_ODE( : , BUTANE) ./ fxns.F_sep;
901                 % fxns.x_ethane_sep = F_soln_ODE( : , ETHANE) ./ fxns.F_sep;
```

```matlab
902                     % fxns.x_water_sep = fxns.F_steam ./ fxns.F_sep;
903
904                     % plot_conversion_fxns(fxns);
905
906
907
908
909                     % Debugging
910                     if CASHFLOW_MATRIX_OUTPUT
911                         fprintf("\n\nnpv = ($ MM) %3.3f \n", ideal_lifetimeNpv)
912                         format short
913                         % disp(ideal_cf.matrix)
914
915                         disp(ideal_params)
916                         fprintf("conversion = %1.4f\n", ideal_conversion)
917
918                         A = [123456789, 987654321; 12345, 67890]; % Example 2D array
919
920                         % Loop through each element and print
921                         disp("CASH FLOW MATRIX")
922                         A = ideal_cf.matrix;
923                         [row, col] = size(A);
924                         for i = 1:row
925                             for j = 1:col
926                                 fprintf('%6.1f\t', A(i,j)); % Adjust the format↙
specifier as needed
927                             end
928                             fprintf('\n');
929                         end
930
931                         % cf.matrix
932                         % cf.lifetime_npv
933                     end
934
935
936
937                 %↙
PLOTTING_____
938                 col_names = {'V_rxtr [L] ', 'Hydrogen [kta]', 'Methane', ...
939                     'Ethylene', 'Propane', 'Butane','Ethane', 'conversion', ...
940                     'S1', 'S2', 'q0 [ L /s ]', 'Vol_plant [ L ]', 'q0 plant', 'cost↙
reactor', 'profit', 'net profit', 'conserv mass', 'npv', 'separationCosts', 'Furnace↙
Costs'};
941                 soln_table = table( V_soln_ODE, F_soln_ODE(:, HYDROGEN), ...
942                         F_soln_ODE(:, METHANE), F_soln_ODE(:, ETHYLENE), ...
943                         F_soln_ODE(:, PROPANE), F_soln_ODE(:, BUTANE), ...
944                         F_soln_ODE(:, ETHANE), conversion,select_1, ...
945                         select_2,q0,V_plant,q0_plant,cost_rxt_vec,profit, profit↙
- cost_rxt_vec, conserv_mass,npv,fxns.separationCosts,fxns.furnaceCosts,'VariableNames',↙
col_names)
946                 soln_table.Properties.VariableNames = col_names;
947
948                 % Computer Selectivity vs conversion relationships
949
950                 % Use Selectivity vs Conversion Relationships with lvl 2 & 3↙
balances
951                 % % to calculate the true feed flow rates into the reactor
952
```

```matlab
953                    % % ?? MODIFY ALL OF THESE TO BE IN MILLIONS OF DOLLARS
954                    % npv.mainProductRevenue = value_ethylene(P_ethylene);
955                    % npv.byProductRevenue = value_h2_chem(P_hydrogen -↙
combusted_hydrogen);
956                    % npv.rawMaterialsCost = value_ethane(F_fresh_ethane);
957                    % npv.utilitiesCost = cost_steam(F_steam, COST_RATES_STEAM↙
(STEAM_CHOICE, STEAM_COST_COL));
958                    % npv.CO2sustainabilityCharge = tax_C02(combusted_fuel_flow_rates,↙
F_natural_gas);
959                    % npv.conversion = conversion(i);
960                    % npv.ISBLcapitalCost = cost_rxt_vec + cost_separation_system↙
(P_flowrates, F_steam, R_ethane);
961                    % % NPV CALCS
962
963                k = k + 1;
964              end
965          j = j + 1;
966         end
967      i = i + 1;
968      end
969 end
970
971 % Plotting the Capstone plots
972
973 fxns.conversion = conversion;
974 fxns.V_plant = V_plant;
975 fxns.select_1 = select_1;
976 fxns.select_2 = select_2;
977 fxns.npv = npv;
978 fxns.recycle = F_soln_ODE( : , ETHANE);
979 fxns.freshFeedRawMaterials = fxns.F_fresh_ethane + fxns.F_steam;
980 fxns.productionRateRxnProducts = F_soln_ODE( : , HYDROGEN : BUTANE);
981 fxns.F_rxtr_in_total = fxns.F_fresh_ethane + fxns.recycle + fxns.F_steam;
982 fxns.F_sep = sum(F_soln_ODE(: , HYDROGEN : ETHANE), 2) + fxns.F_steam;
983 fxns.x_hydrogen_sep = F_soln_ODE( : , HYDROGEN) ./ fxns.F_sep;
984 fxns.x_methane_sep = F_soln_ODE( : , METHANE) ./ fxns.F_sep;
985 fxns.x_ethylene_sep = F_soln_ODE( : , ETHYLENE) ./ fxns.F_sep;
986 fxns.x_propane_sep = F_soln_ODE( : , PROPANE) ./ fxns.F_sep;
987 fxns.x_butane_sep = F_soln_ODE( : , BUTANE) ./ fxns.F_sep;
988 fxns.x_ethane_sep = F_soln_ODE( : , ETHANE) ./ fxns.F_sep;
989 fxns.x_water_sep = fxns.F_steam ./ fxns.F_sep;
990 fxns.npv_T_P_MR = npv_T_P_MR;
991
992 plot_conversion_fxns(fxns);
993
994
995
996 disp("The Script is done running  ')
997 % HELPER FUNCTIONS | PLOTTING_____
998
999 function z = plot_contour(x, y, z, options)
1000    global PSA_TOGGLE
1001    % Unpack options
1002    x_label = options{1};
1003    y_label = options{2};
1004    plt_title = options{3};
1005    plt_saveName = options{4};
1006
```

```matlab
1007        if PSA_TOGGLE
1008            stringValue = 'true';
1009        else
1010            stringValue = 'false';
1011        end
1012        plt_title = plt_title + sprintf(" PSA %s ", stringValue);
1013
1014        hold on
1015        figure
1016        [C, h] = contourf(x, y, z); % Create filled contours
1017        clabel(C, h,  'FontSize', 10, 'Color', 'k', 'LabelSpacing', 200); % Customize↙
label properties
1018        xlabel(x_label);
1019        ylabel(y_label);
1020        title(plt_title);
1021        saveas(gcf, plt_saveName);
1022        hold off
1023 end
1024
1025 function plot_3D(x, y, z, options)
1026        global PSA_TOGGLE
1027
1028        % Unpack options
1029        x_label = options{1};
1030        y_label = options{2};
1031        plt_title = options{3};
1032        plt_saveName = options{4};
1033
1034        if PSA_TOGGLE
1035            stringValue = 'true';
1036        else
1037            stringValue = 'false';
1038        end
1039        plt_title = plt_title + sprintf(" PSA %s ", stringValue);
1040
1041         % Create a new figure
1042        hold on; % Hold on to add multiple plot elements
1043        figure
1044        surf(x, y, z); % Create a 3D surface plot
1045
1046        % Customizing the plot
1047        xlabel(x_label);
1048        ylabel(y_label);
1049        zlabel('Z Value'); % Add a label for the z-axis
1050        title(plt_title);
1051        colorbar; % Adds a color bar to indicate the scale of z values
1052 %      shading interp; % Option for smoother color transition on the surface
1053
1054        hold off; % Release the figure
1055        saveas(gcf, plt_saveName); % Save the figure to file
1056 end
1057
1058
1059 function plotFlowRatesForRow(row, flowRatesArray)
1060        % flowRatesArray is expected to be an array of matrices, where each matrix↙
corresponds to a species' flow rates
1061
1062        % Names of the gases for labeling purposes
```

```matlab
1063        gasNames = {'Hydrogen', 'Methane', 'Ethylene', 'Propane', 'Butane', 'Ethane'};
1064
1065        % Create a figure
1066        figure;
1067        hold on; % Hold on to plot all data on the same figure
1068
1069        % Loop through each flow rate matrix in the array
1070        for i = 1:length(flowRatesArray)
1071            % Extract the specified row from the current matrix
1072            currentRow = flowRatesArray{i}(row, :);
1073
1074            % Plot the current row with a marker
1075            plot(currentRow, '-o', 'DisplayName', gasNames{i});
1076        end
1077
1078        % Adding plot features
1079        title(sprintf('Flow Rates for Row %d', row));
1080        xlabel('Selectivity 1 (S2 fixed)');
1081        ylabel('Flow Rate');
1082        legend('show');
1083        hold off; % Release the figure for other plots
1084 end
1085
1086 % HELPER FUNCTIONS | HEAT _____
1087
1088 function [combusted_fuel_flowrates, heatflux_left] = fuel_combustion(heat_flux,↙
flowrates)
1089        global HYDROGEN METHANE ETHYLENE PROPANE BUTANE;
1090        global ENTHALPY_METHANE ENTHALPY_PROPANE ENTHALPY_BUTANE HEAT_CAPACITY_ETHANE;
1091        global MT_PER_KT G_PER_KT GJ_PER_KJ KJ_PER_GJ MOLMASS_METHANE KT_PER_G↙
MOLMASS_BUTANE ...
1092                MOLMASS_PROPANE PSA_TOGGLE ENTHALPY_HYDROGEN MOLMASS_HYDROGEN
1093
1094        % Note! : Longest Chain Hydrocarbons are cheapest to combust
1095
1096        % initialize all values in the array to be zero
1097        combusted_fuel_flowrates = flowrates * 0;
1098
1099        % LOGIC : Goes through each heat source in order, returns if the heat flux↙
supplied is sufficient.
1100        heatflux_left = heat_flux;
1101
1102        % (GJ / yr)          = (kt / yr)          * (g / kt) * (kJ / g)         * (GJ /↙
kJ)
1103        Q_combust_all_hydrogen = flowrates(HYDROGEN) * G_PER_KT * ENTHALPY_HYDROGEN *↙
GJ_PER_KJ;
1104
1105        if (~PSA_TOGGLE)
1106            % Hydrogen
1107            if (heatflux_left > Q_combust_all_hydrogen)
1108                combusted_fuel_flowrates(HYDROGEN) = flowrates(HYDROGEN);
1109                heatflux_left = heatflux_left - Q_combust_all_hydrogen;
1110            else
1111                % (kt / yr)                        = ((GJ)                  ) * (KJ / GJ)↙
*
1112                combusted_fuel_flowrates(HYDROGEN) = (heatflux_left) * KJ_PER_GJ * ...
1113                    ... % (mol / KJ)         * (g / mol)         * (kt / g)
1114                    ( 1 / ENTHALPY_HYDROGEN) * MOLMASS_HYDROGEN * KT_PER_G;
```

```matlab
1115            heatflux_left = 0;
1116            return
1117        end
1118    end
1119
1120    % (GJ / yr)             = (kt / yr)         * (g / kt) * (kJ / g)      * (GJ /↵
kJ)
1121    Q_combust_all_methane = flowrates(METHANE) * G_PER_KT * ENTHALPY_METHANE *↵
GJ_PER_KJ;
1122
1123    % Methane
1124    if (heatflux_left > Q_combust_all_methane)
1125        combusted_fuel_flowrates(METHANE) = flowrates(METHANE);
1126        heatflux_left = heatflux_left - Q_combust_all_methane;
1127    else
1128        % (kt / yr)                         = ((GJ)              ) * (KJ / GJ) *
1129        combusted_fuel_flowrates(METHANE) = (heatflux_left) * KJ_PER_GJ * ...
1130            ... % (mol / KJ)       * (g / mol)      * (kt / g)
1131            ( 1 / ENTHALPY_METHANE) * MOLMASS_METHANE * KT_PER_G;
1132        heatflux_left = 0;
1133        return
1134    end
1135
1136    % (GJ / yr)             = (kt / yr)         * (g / kt) * (kJ / g)      * (GJ /↵
kJ)
1137    Q_combust_all_propane = flowrates(PROPANE) * G_PER_KT * ENTHALPY_PROPANE *↵
GJ_PER_KJ;
1138
1139    % Propane
1140    if (heatflux_left > Q_combust_all_propane)
1141        combusted_fuel_flowrates(PROPANE) = flowrates(PROPANE);
1142        heatflux_left = heatflux_left - Q_combust_all_propane;
1143    else
1144        % (kt / yr)                         = ((GJ)              ) * (KJ / GJ) *
1145        combusted_fuel_flowrates(PROPANE) = (heatflux_left) * KJ_PER_GJ * ...
1146            ... % (mol / KJ)       * (g / mol)      * (kt / g)
1147            ( 1 / ENTHALPY_PROPANE) * MOLMASS_PROPANE * KT_PER_G;
1148        heatflux_left = 0;
1149        return
1150    end
1151
1152    % (GJ / yr)             = (kt / yr)         * (g / kt) * (kJ / g)      * (GJ /↵
kJ)
1153    Q_combust_all_butane = flowrates(BUTANE) * G_PER_KT * ENTHALPY_BUTANE *↵
GJ_PER_KJ;
1154
1155    % Butane
1156    if (heatflux_left > Q_combust_all_butane)
1157        combusted_fuel_flowrates(BUTANE) = flowrates(BUTANE);
1158        heatflux_left = heatflux_left - Q_combust_all_butane;
1159    else
1160        % (kt / yr)                         = ((GJ)              ) * (KJ / GJ) *
1161        combusted_fuel_flowrates(BUTANE) = (heatflux_left) * KJ_PER_GJ * ...
1162            ... % (mol / KJ)       * (g / mol)      * (kt / g)
1163            ( 1 / ENTHALPY_BUTANE) * MOLMASS_BUTANE * KT_PER_G;
1164        heatflux_left = 0;
1165        return
1166    end
```

```matlab
1167 end
1168
1169 %         GJ    =                (kta   , __         , bar      , C )
1170 function heat = heat_steam(F_steam, STEAM_CHOICE, P_reactor, T_reactor)
1171     global COST_RATES_STEAM;
1172     global STEAM_PRESSURE_COL STEAM_TEMP_COL COST_RATES_STEAM G_PER_KT ...
1173         MOLMASS_WATER BAR_PER_PSIA C_TO_K HEAT_CAPACITY_WATER GJ_PER_KJ;
1174
1175     P_steam = COST_RATES_STEAM(STEAM_CHOICE, STEAM_PRESSURE_COL); % [ psia ]
1176     T_steam = COST_RATES_STEAM(STEAM_CHOICE, STEAM_TEMP_COL);    % [ C ]
1177     P_steam = P_steam * BAR_PER_PSIA;
1178     T_steam = T_steam + C_TO_K;
1179     T_reactor = T_reactor + C_TO_K;
1180
1181     if (P_steam > P_reactor) % Adiabatic Expansion
1182         T_adibatic = (T_steam) * (P_reactor / P_steam);
1183         T_steam = T_adibatic;
1184     elseif (P_steam < P_reactor) % Compression
1185         W = compressor_work(T_reactor, P_steam, P_reactor);
1186         if ADD_COMPRESSOR_WORK_TO_STEAM_HEATFLUX
1187             heat = heat + W;
1188         end
1189         % I should add this to the heat flux probably ??
1190     end
1191
1192     % KJ = kta    * (G / KT) * (mol / g)        * (KJ / MOL K)       * (K - K)
1193     heat = F_steam * G_PER_KT * (1/MOLMASS_WATER) * HEAT_CAPACITY_WATER * (T_reactor↙
- T_steam);
1194     % GJ = KJ   * (KJ / GJ)
1195     heat = heat * GJ_PER_KJ;
1196
1197
1198     % Heat flux after temperture
1199
1200
1201
1202 end
1203
1204 function T_f = adiabatic_temp(T_0, P_0, P_f)
1205
1206     T_f = T_0 * ( P_0 / P_f);
1207 end
1208
1209 function W = compressor_work(T, P_0, P_f)
1210     R = 8.314;      % [ J / mol K]
1211
1212     W = - n * R * T * log(P_f / P_0);
1213
1214     % ?? THIS ALWAYS RETURNS 0 OR NULL, NOT IMPLEMENTED YET
1215
1216 end
1217
1218 % HELPER FUNCTIONS | TAXES_____
1219
1220 function cost = tax_C02(combusted_flowrates, F_natural_gas)
1221     global HYDROGEN METHANE ETHYLENE PROPANE BUTANE TAX_CO2_PER_MT;
1222     global MT_CO2_PER_KT_METHANE MT_CO2_PER_KT_PROPANE MT_CO2_PER_KT_BUTANE ...
1223     MT_CO2_PER_KT_NATURALGAS;
```

```matlab
1224
1225     % Calculate the cost per kt (in tax) of each combusted fuel
1226     methane = combusted_flowrates(METHANE);
1227     propane = combusted_flowrates(PROPANE);
1228     butane = combusted_flowrates(BUTANE);
1229
1230     mt_c02 = 0;
1231     % kta  =  (MT)  + ( (kt fuel / yr) * (MT CO2 / KT FUEL) )
1232     mt_c02 = mt_c02 + methane * MT_CO2_PER_KT_METHANE;
1233     mt_c02 = mt_c02 + propane * MT_CO2_PER_KT_PROPANE;
1234     mt_c02 = mt_c02 + butane * MT_CO2_PER_KT_BUTANE;
1235     mt_c02 = mt_c02 + F_natural_gas * MT_CO2_PER_KT_NATURALGAS;
1236
1237     cost = mt_c02 * TAX_CO2_PER_MT;
1238 end
1239
1240 % HELPER FUNCTIONS | FUEL COSTS_____
1241
1242 function cost = cost_natural_gas_fuel(heat_flux_remaining)
1243     global VALUE_NATGAS_FUEL
1244     % $ / yr = (GJ)          * ($ / GJ)
1245     cost = heat_flux_remaining * VALUE_NATGAS_FUEL;
1246 end
1247
1248 % HELPER FUNCTIONS | FUEL FLOWRATES_____
1249
1250 function F_natural_gas = natgas_combustion(heat_flux_remaining)
1251     global KJ_PER_GJ ENTHALPY_NAT_GAS KT_PER_G MOLMASS_NATGAS;
1252     % output should be in kta, input is in GJ
1253
1254     %       kt          GJ             * (kJ / GJ) * (mol / kJ) *      (g /↙
mol) *          (kt / g)
1255     F_natural_gas = heat_flux_remaining * KJ_PER_GJ * (1/ENTHALPY_NAT_GAS) *↙
(MOLMASS_NATGAS) * KT_PER_G;
1256
1257 end
1258
1259 % FUNCTIONS | REACTOR ODE SYSTEM_____
1260
1261 function dFdV = reactionODEs(V, F, T, P, F_steam)
1262     global R_2 k1_f k1_r k2 k3 C_TO_K MOLMASS_METHANE MOLMASS_ETHANE↙
MOLMASS_ETHYLENE ...
1263         MOLMASS_PROPANE MOLMASS_HYDROGEN MOLMASS_BUTANE YR_PER_SEC G_PER_KT↙
SEC_PER_YR KT_PER_G
1264     % INPUT UNITS
1265     % V [ L ]
1266     % F [ kta ]
1267     % T [ Celcius ]
1268     % P [ bar ]
1269
1270     % Change the input units so that evrything is consistent
1271     % P = P * ATM_PER_BAR;
1272     T = T + C_TO_K;
1273
1274     % Product flow rate indicies
1275     HYDROGEN = 1;
1276     METHANE = 2;
1277     ETHYLENE = 3;
```

```matlab
1278        PROPANE = 4;
1279        BUTANE = 5;
1280
1281        % Feed flow rate index
1282        ETHANE = 6;
1283
1284        F_tot = sum(F) + F_steam;
1285
1286
1287        % Hydrogen = A
1288        dFAdV = (k1_f(T) * ( (F(ETHANE) * P) / (F_tot * R_2 * T) )   ) - ...
1289                (k1_r(T) * ( F(ETHYLENE) * F(HYDROGEN) * P^2) ) / (F_tot * R_2 * T)^2;
1290
1291        % Methane = B
1292        dFBdV = (k2(T) * (F(ETHANE) * P)^2) / (F_tot * R_2 * T)^2;
1293
1294        % Ethylene = C
1295        dFCdV = (k1_f(T) * (F(ETHANE) * P / (F_tot * R_2 * T))) - ...
1296                (k1_r(T) * (F(ETHYLENE) * F(HYDROGEN) * P^2) / (F_tot * R_2 * T)^2) -↙
...
1297                (k3(T) * (F(ETHANE) * F(ETHYLENE) * P^2) / (F_tot * R_2 * T)^2);
1298
1299        % Propane = E
1300        dFEdV = k2(T) * (F(ETHANE) * P)^2 / (F_tot * R_2 * T)^2;
1301
1302        % Butane = F
1303        dFFdV = (k3(T) * (F(ETHANE) * F(ETHYLENE) * P^2)) / (F_tot * R_2 * T)^2;
1304
1305        % Ethane = D
1306        dFDdV = (-k1_f(T) * (F(ETHANE) * P / (F_tot * R_2 * T))) + ...
1307                (k1_r(T) * (F(ETHYLENE) * F(HYDROGEN) * P^2)/(F_tot * R_2 * T)^2) - ...
1308                (k2(T) * F(ETHANE)^2 * P^2 / (F_tot * R_2 * T)^2) - ...
1309                (k3(T) * F(ETHANE) * F(ETHYLENE) * P^2 / (F_tot * R_2 * T)^2);
1310
1311        T = T - C_TO_K;
1312
1313        dFdV = [dFAdV; dFBdV; dFCdV; dFEdV; dFFdV; dFDdV];
1314
1315 end
1316
1317 function cost = cost_reactor(V_plant_input)
1318        global FT_PER_METER STEAM_TO_FEED_RATIO
1319        FT_PER_METER = 3.28084;
1320        % ??? WHAT ARE THE UNITS OF TIME
1321        %
1322        pi = 3.14159;
1323        D = 0.05;                               % [m]
1324        V_plant_max = pi * (0.025)^2 * 20;      %[m^3]
1325
1326        % Reactors have a max length, so calculate the number of full size reactors
1327        % and add it to the cost of the one non-max length reactor
1328
1329        cost = 0;
1330
1331        % Find the Cost of the max-sized reactors
1332        num_of_additional_reactors = int64(V_plant_input / V_plant_max);
1333        num_of_additional_reactors = double(num_of_additional_reactors);
1334
```

```matlab
1335        V_plant = V_plant_max;
1336        factor_1 = 4.18;
1337        factor_2 = (V_plant / (pi * (D/2)^2) * FT_PER_METER)^0.82;
1338        factor_3 = (101.9 * D * FT_PER_METER)^1.066;
1339        factor_4 = (1800 / 280);
1340        cost_max_reactor = factor_1 * factor_2 * factor_3 * factor_4;
1341        cost = cost + num_of_additional_reactors * cost_max_reactor;
1342
1343
1344        % Find the cost of the non-max size reactor
1345        V_plant = V_plant_input - V_plant_max * num_of_additional_reactors;
1346        if V_plant < 0
1347            V_plant = 0;
1348        end
1349        factor_1 = 4.18;
1350        factor_2 = (V_plant / (pi * (D/2)^2) * FT_PER_METER)^0.82;
1351        factor_3 = (101.9 * D * FT_PER_METER)^1.066;
1352        factor_4 = (1800 / 280);
1353        cost = cost + factor_1 * factor_2 * factor_3 * factor_4;
1354
1355
1356 end
1357
1358 %         [$]   =                   ( kta   )
1359 function cost = cost_waste_stream(F_steam)
1360     global MOLMASS_WATER G_PER_KT YR_PER_SEC R_2 M3_PER_L T_SEPARATION ...
1361             P_SEPARATION SEC_PER_YR C_TO_K DENSITY_LIQ_WATER KG_PER_KT
1362
1363     % m^3 / s = (kt / yr) * (kg / kt)   * (m^3 / kg)  * (yr / s)
1364     q = F_steam * KG_PER_KT * (1 / DENSITY_LIQ_WATER) * YR_PER_SEC;
1365         % ?? Assume that all of the water out of the sep system is liquid
1366
1367     a = 0.001 + 2e-4*q^(-0.6);
1368         %Source: Uldrich and Vasudevan
1369     b=0.1;
1370         %Source: Uldrich and Vasudevan
1371     CEPCI = 820;
1372         %Source: Lecture slides
1373     C_f = 3.0;                      % [ $ / GJ ]
1374
1375     %$/m^3 waste water
1376     cost_waste_water = a*CEPCI + b*C_f;
1377
1378     % m^3 / s = (m^3 / s) * (s / yr)
1379     q = q * SEC_PER_YR;
1380     cost = cost_waste_water * q;
1381
1382 end
1383
1384 function cost = cost_separation_system(P_flowrates, F_steam, R_ethane)
1385     global MOLMASS_METHANE MOLMASS_HYDROGEN MOLMASS_ETHANE MOLMASS_ETHYLENE ...
1386         MOLMASS_PROPANE MOLMASS_BUTANE YR_PER_SEC
1387     global T_SEPARATION R PRESS_RXTR R ...
1388      MAX_OPEX MAX_TFCI MAX_CAPEX G_PER_KT MOLMASS_WATER
1389
1390     % Product flow rate indicies
1391     HYDROGEN = 1;
1392     METHANE = 2;
```

```matlab
1393        ETHYLENE = 3;
1394        PROPANE = 4;
1395        BUTANE = 5;
1396
1397        % Feed flow rate index
1398        ETHANE = 6;
1399
1400        % SEPARATION_EFFICIENCY_FACTOR = 30;
1401        T = T_SEPARATION; % [ K ]
1402
1403        %Using compositions from ASPEN
1404        %Component mole flow rate out of rxtr over total mole flow rate out of reactor
1405        % Mol fractions out of the reactoor
1406
1407        % (mol / s) = (kt / yr) * (g / kt) * (mol / g) * (yr / s)
1408        P_flowrates(METHANE) = P_flowrates(METHANE) * G_PER_KT * (1/MOLMASS_METHANE) *↵
YR_PER_SEC;
1409        P_flowrates(HYDROGEN) = P_flowrates(HYDROGEN) * G_PER_KT * (1/MOLMASS_HYDROGEN)↵
* YR_PER_SEC;
1410        R_ethane = R_ethane * G_PER_KT * (1/MOLMASS_ETHANE) * YR_PER_SEC;
1411        P_flowrates(ETHYLENE) = P_flowrates(ETHYLENE) * G_PER_KT * (1/MOLMASS_ETHYLENE)↵
* YR_PER_SEC;
1412        P_flowrates(PROPANE) = P_flowrates(PROPANE) * G_PER_KT * (1/MOLMASS_PROPANE) *↵
YR_PER_SEC;
1413        P_flowrates(BUTANE) = P_flowrates(BUTANE) * G_PER_KT * (1/MOLMASS_BUTANE) *↵
YR_PER_SEC; % Add this line for butane
1414        F_steam = F_steam * G_PER_KT * (1/MOLMASS_WATER) * YR_PER_SEC;
1415
1416        %CONVERT TO_MOLES
1417
1418        P_tot = sum(P_flowrates(HYDROGEN:BUTANE)) + F_steam + R_ethane;
1419
1420        z_methane = P_flowrates(METHANE) / P_tot;
1421        z_hydrogen = P_flowrates(HYDROGEN) / P_tot;
1422        z_ethane = R_ethane / P_tot;
1423        z_ethylene = P_flowrates(ETHYLENE) / P_tot;
1424        z_propane = P_flowrates(PROPANE) / P_tot;
1425        z_butane = P_flowrates(BUTANE) / P_tot;
1426        z_water = F_steam / P_tot;
1427
1428        %Mol fractions leaving each separation system (refer to Isa's drawing in GN)
1429        % leaving sep 1
1430        x_water = 1;
1431
1432        % leaving sep 4
1433        x_ethane = 1;
1434        x_ethylene = 1;
1435
1436        % leaving sep 2
1437        x_butane = 0.0003;
1438        x_propane = 1 - x_butane;
1439
1440        % leaving sep 5 (PSA)
1441        x_methane = 4.03293090303065e-004;
1442        x_hydrogen = 1 - x_methane;
1443            % ?? How should I implement the PSA toggle switch on this
1444
1445        %Pressures of PSA system [bar]
```

```matlab
1446        P_in = PRESS_RXTR;
1447        P_H2 = 10;               % [ bar ]
1448        P_ME = 1;                % [ bar ]
1449           % These outlet pressures are constant for PSA system. DONT change
1450
1451        %Using flow rates from ASPEN [NOTE: FOR MATLAB USE THE VALUES FROM THE
1452        %SOLN_TABLE. WE USED THESE AS EXPECTED COSTS)
1453
1454        % Flowrates of each exiting stream from the sep system
1455
1456        F_water = F_steam;                              % mol/s
1457        F_LPG = P_flowrates(BUTANE) + P_flowrates(PROPANE); % (mol / s)
1458        F_ethylene = P_flowrates(ETHYLENE);             % (mol / s)
1459        F_ethane = R_ethane;                      % (mol / s)
1460        F_H2 = P_flowrates(HYDROGEN);                   % (mol / s)
1461        F_ME = P_flowrates(METHANE);                    % (mol / s);
1462
1463    %(J/s) =    (mol/s) * (J/mol K) * (T)
1464    W_min_Sep_System = F_water*R*T*log(x_water/z_water) + ...
1465                    F_LPG*R*T*log(x_propane/z_propane + ...
1466                              x_butane/z_butane) + ...
1467                    F_ethylene*R*T*log(x_ethylene/z_ethylene) + ...
1468                    F_ethane*R*T*log(x_ethane/z_ethane) + ...
1469                    R*T*( ...
1470                        F_H2*log(P_H2/P_in)+ ...
1471                        F_H2*log(x_hydrogen/z_hydrogen) +...
1472                        F_ME*log(x_methane/z_methane) +...
1473                        F_ME*log(P_ME/P_in)...
1474                        );
1475
1476
1477        lamdba_min = 20;
1478        lambda_max = 50;
1479        cost_energy = 3;          % ( $ / GJ )
1480
1481        if MAX_OPEX
1482    %($/yr)              =    (J/s)      * (GJ/J) * (Work Efficiency) *($/GJ)* (s/yr)
1483            opex =  W_min_Sep_System*1e-9 * lambda_max * cost_energy * 30.24e6;
1484        else
1485            opex = W_min_Sep_System*1e-9 * lamdba_min * cost_energy * 30.24e6;
1486        end
1487
1488        if MAX_CAPEX
1489    %($)                   = ($/W)    (Efficiency) * (J/s)
1490            capex = 1 * lambda_max * W_min_Sep_System;
1491        else
1492            capex = 0.5 * lamdba_min * W_min_Sep_System;
1493        end
1494
1495        cost = 2.5 * capex ;
1496
1497 end
1498
1499
1500 function cf = get_npv(npv)
1501     global YEARS_IN_OPERATION
1502     % USER_INPUTS | All inputs are in units of $MM
1503         % npv.mainProductRevenue = value_ethylene(P_ethylene);
```

```matlab
1504            % npv.byProductRevenue = value_h2_chem(P_hydrogen - combusted_hydrogen);
1505            % npv.rawMaterialsCost = value_ethane(F_fresh_ethane);
1506            % npv.utilitiesCost = cost_steam(F_steam, COST_RATES_STEAM(STEAM_CHOICE,↙
STEAM_COST_COL));
1507            % npv.CO2sustainabilityCharge = tax_C02(combusted_fuel_flow_rates,↙
F_natural_gas);
1508            % npv.conversion = conversion(i);
1509            % npv.isbl = cost_rxt_vec + cost_separation_system(P_flowrates, F_steam,↙
R_ethane);
1510
1511        WORKING_CAP_PERCENT_OF_FCI = 0.15;        % [ % in decimal ]
1512        STARTUP_COST_PERCENT_OF_FCI = 0.10;       % [ % in decimal ]
1513        LENGTH_CONSTRUCTION_TABLE = 6;
1514        LAST_ROW_CONSTRUCTION = LENGTH_CONSTRUCTION_TABLE;
1515        YEARS_OF_CONSTUCTION = 3;
1516
1517        % Revenues & Production Costs
1518        npv.consummablesCost = 0;
1519        npv.VCOP = npv.rawMaterialsCost + npv.utilitiesCost + ...
1520                    npv.consummablesCost + npv.CO2sustainabilityCharge - ...
1521                                            npv.byProductRevenue;
1522        npv.salaryAndOverhead = 0;
1523        npv.maintenenace = 0;
1524        npv.interest = 15;
1525        npv.AGS = (npv.mainProductRevenue + npv.byProductRevenue)*0.05;     % ~5%↙
revenue
1526        npv.FCOP = npv.salaryAndOverhead + npv.maintenenace +...
1527                        npv.AGS + npv.interest;
1528
1529        % Capital Costs
1530        npv.OSBLcapitalCost = npv.ISBLcapitalCost * 0.40;
1531        npv.contingency = (npv.ISBLcapitalCost + npv.OSBLcapitalCost) * 0.25;
1532        npv.indirectCost = (npv.ISBLcapitalCost + npv.OSBLcapitalCost + ...
1533                                            npv.contingency) * 0.30;
1534        npv.totalFixedCapitalCost = npv.ISBLcapitalCost + ...
1535                                    npv.OSBLcapitalCost + ...
1536                                    npv.indirectCost + ...
1537                                    npv.contingency;
1538
1539        npv.workingCapital = npv.totalFixedCapitalCost * WORKING_CAP_PERCENT_OF_FCI;
1540        npv.startupCost = npv.totalFixedCapitalCost * STARTUP_COST_PERCENT_OF_FCI;
1541        npv.land = 10;
1542        npv.totalCapitalInvestment = npv.totalFixedCapitalCost + ...
1543                                        npv.workingCapital + ...
1544                                        npv.startupCost + ...
1545                                        npv.land;
1546        % Economic Assumptions
1547        npv.discountRate = 0.15;        % [ % in decimal ]
1548        npv.taxRate = 0.27;             % [ % in decimal ]
1549        npv.salvageValue = 0.05;        % [ % in decimal ]
1550
1551        % CONSTRUCTION SCHEDULE INDICIES
1552        YEAR = 1;
1553        FC = 2;
1554        WC = 3;
1555        SU = 4;
1556        FCOP = 5;
1557        VCOP = 6;
```

```matlab
1558        construction_matrix = zeros(LENGTH_CONSTRUCTION_TABLE + 1, VCOP);
1559
1560        % Generate the construction schedule matrix
1561        for yr = 0:LENGTH_CONSTRUCTION_TABLE
1562            row = yr + 1;
1563            if yr > 0 && yr < 4
1564                construction_matrix(row, FC) = 0.33;
1565            end
1566            if yr == 3
1567                construction_matrix(row, WC) = 1.00;
1568                construction_matrix(row, SU) = 1.00;
1569            end
1570            if yr > 3 && yr <= 6
1571                construction_matrix(row, FCOP) = 1.00;
1572                construction_matrix(row, VCOP) = 1.00;
1573            end
1574        end
1575
1576        % NPV COLUMN INDICIES
1577        YEAR = 1;
1578        CAPITAL_EXPENSE = 2;
1579        REVENUE = 3;
1580        COM = 4;
1581        GROSS_PROFIT = 5;
1582        DEPRECIATION = 6;
1583        TAXABLE_INC = 7;
1584        TAXES_PAID = 8;
1585        CASH_FLOW = 9;
1586        CUM_CASH_FLOW = 10;
1587        PV_OF_CF = 11;
1588        CUM_PV_OF_CF = 12;
1589        NPV = 13;
1590        cash_flow_matrix = zeros(YEARS_IN_OPERATION + 1, NPV);
1591        LAST_ROW_CASHFLOW = YEARS_IN_OPERATION + 1;
1592
1593
1594        for yr = 0:YEARS_IN_OPERATION
1595            row = yr + 1;
1596            cash_flow_matrix(row, YEAR) = yr;
1597
1598            % Capital Expenses Column
1599            if yr == 0
1600                cash_flow_matrix(row, CAPITAL_EXPENSE) = npv.land;
1601            elseif yr >= 1 && yr <= 5
1602                cash_flow_matrix(row, CAPITAL_EXPENSE) ...
1603                    = npv.totalFixedCapitalCost * construction_matrix(row,FC) + ...
1604                    npv.workingCapital * construction_matrix(row, WC) + ...
1605                    npv.startupCost * construction_matrix(row, SU) ;
1606            elseif yr == YEARS_IN_OPERATION
1607                cash_flow_matrix(row, CAPITAL_EXPENSE) = - npv.salvageValue * npv.↵
totalFixedCapitalCost;
1608            else
1609                cash_flow_matrix(row, CAPITAL_EXPENSE) ...
1610                    = npv.totalFixedCapitalCost * construction_matrix↵
(LAST_ROW_CONSTRUCTION,FC) + ...
1611                    npv.workingCapital * construction_matrix(LAST_ROW_CONSTRUCTION,↵
WC) + ...
1612                    npv.startupCost * construction_matrix(LAST_ROW_CONSTRUCTION, SU) ;
```

```matlab
1613          end
1614
1615          % Revenue Column
1616          if yr <= LENGTH_CONSTRUCTION_TABLE % ??
1617              cash_flow_matrix(row, REVENUE) = npv.mainProductRevenue *↙
construction_matrix(row, VCOP);
1618          else
1619              cash_flow_matrix(row, REVENUE) = npv.mainProductRevenue *↙
construction_matrix(LAST_ROW_CONSTRUCTION, VCOP);
1620          end
1621
1622          % COM Column
1623          if yr <= LENGTH_CONSTRUCTION_TABLE
1624              cash_flow_matrix(row, COM) = npv.VCOP * construction_matrix(row, VCOP) +↙
...
1625                                           npv.FCOP * construction_matrix(row,↙
FCOP);
1626          else
1627              cash_flow_matrix(row, COM) = npv.VCOP * construction_matrix↙
(LAST_ROW_CONSTRUCTION, VCOP) + ...
1628                                           npv.FCOP * construction_matrix↙
(LAST_ROW_CONSTRUCTION, FCOP);
1629          end
1630
1631          % Gross Profit
1632          cash_flow_matrix(row, GROSS_PROFIT) = cash_flow_matrix(row,REVENUE) -↙
cash_flow_matrix(row, COM);
1633
1634          % Depreciation
1635          if yr >= YEARS_OF_CONSTUCTION
1636              cash_flow_matrix(row, DEPRECIATION) = 0.1*(npv.totalFixedCapitalCost +↙
npv.startupCost - 0.05*npv.totalFixedCapitalCost);
1637          end
1638
1639          % Taxable Inc
1640          if yr >= YEARS_OF_CONSTUCTION
1641              cash_flow_matrix(row, TAXABLE_INC) = cash_flow_matrix(row, GROSS_PROFIT)↙
- cash_flow_matrix(row,DEPRECIATION);
1642          end
1643
1644          % Taxes Paid
1645          if yr >= YEARS_OF_CONSTUCTION
1646              cash_flow_matrix(row, TAXES_PAID) = cash_flow_matrix(row, TAXABLE_INC) *↙
npv.taxRate;
1647          end
1648
1649          % Cash Flow
1650          cash_flow_matrix(row, CASH_FLOW) = -cash_flow_matrix(row, CAPITAL_EXPENSE) +↙
...
1651              ( cash_flow_matrix(row,REVENUE) ...
1652                  - cash_flow_matrix(row, COM) ...
1653                  - cash_flow_matrix(row, DEPRECIATION) ...
1654              ) * ( 1 - npv.taxRate) + cash_flow_matrix(row, DEPRECIATION);
1655
1656          % Cummulative Cash Flow
1657          cash_flow_matrix(row, CUM_CASH_FLOW) = sum( cash_flow_matrix( 1 : row,↙
CASH_FLOW) );
1658
```

```matlab
1659          % PV of CF
1660          cash_flow_matrix(row, PV_OF_CF) = cash_flow_matrix(row, CASH_FLOW) / ( 1 +↵
npv.discountRate)^yr;
1661
1662          % Cummulative PV of CF
1663          cash_flow_matrix(row , CUM_PV_OF_CF) = sum( cash_flow_matrix(1:row,↵
PV_OF_CF) );
1664
1665          % NPV
1666          if row > 1
1667              cash_flow_matrix(row , NPV) = cash_flow_matrix(row - 1, NPV) +↵
cash_flow_matrix(row, PV_OF_CF);
1668          else
1669              cash_flow_matrix(row, NPV) = cash_flow_matrix(row, PV_OF_CF);
1670          end
1671      end
1672
1673      % RETURN
1674      % cash_flow_matrix
1675 %    [cf_matrix, lifetime_npv] = [cash_flow_matrix, cash_flow_matrix↵
(LAST_ROW_CASHFLOW, NPV)];
1676      cf.matrix = cash_flow_matrix;
1677      cf.lifetime_npv = cash_flow_matrix(LAST_ROW_CASHFLOW, NPV);
1678      % lifetime_npv = cash_flow_matrix(LAST_ROW_CASHFLOW, NPV);
1679 end
1680
1681
1682
1683 function installedCost = calculate_installed_cost(Q)
1684      global MILLIONBTU_PER_GJ MILLIONBTU_PER_GJ YR_PER_HR HR_PER_YR
1685
1686      Q = Q * MILLIONBTU_PER_GJ * YR_PER_HR;
1687
1688      % Constants
1689      M_and_S = 1800; % Marshall and Swift index
1690      base_cost = 5.52 * 10^3;
1691
1692      % Purchased cost calculation
1693      % F_c = F_d + F_m + F_p;
1694      F_c = 1.1;
1695
1696      % Installed cost calculation
1697      installedCost = (M_and_S / 280) * (base_cost * Q^0.85 * (1.27 + F_c));
1698
1699      installedCost = installedCost;
1700 end
1701
1702
1703
1704 function void = plot_conversion_fxns(fxns)
1705      global T_OVERRIDE P_OVERRIDE STEAM_MR_OVERRIDE
1706      global M3_PER_L
1707      % USER INPUT
1708          % fxns.conversion = conversion;
1709          % fxns.V_plant = V_plant;
1710          % fxns.select_1 = select_1;
1711          % fxns.select_2 = select_2;
1712          % fxns.npv = npv;
```

```matlab
1713             % fxns.recycle = F_soln_ODE( : , ETHANE);
1714             % fxns.freshFeedRawMaterials = fxns.F_fresh_ethane + fxns.F_steam;
1715             % fxns.productionRateRxnProducts = F_soln_ODE( : , HYDROGEN : BUTANE);
1716             % fxns.F_rxtr_in_total = fxns.F_fresh_ethane + fxns.recycle + fxns.F_steam;
1717             % fxns.F_sep = sum(F_soln_ODE(: , HYDROGEN : ETHANE), 2) + fxns.F_steam;
1718             % fxns.x_hydrogen_sep = F_soln_ODE( : , HYDROGEN) ./ fxns.F_sep;
1719             % fxns.x_methane_sep = F_soln_ODE( : , METHANE) ./ fxns.F_sep;
1720             % fxns.x_ethylene = F_soln_ODE( : , ETHYLENE) ./ fxns.F_sep;
1721             % fxns.x_propane_sep = F_soln_ODE( : , PROPANE) ./ fxns.F_sep;
1722             % fxns.x_butane_sep = F_soln_ODE( : , BUTANE) ./ fxns.F_sep;
1723             % fxns.x_ethane_sep = F_soln_ODE( : , ETHANE) ./ fxns.F_sep;
1724             % fxns.x_water_sep = fxns.F_steam ./ fxns.F_sep;
1725
1726         x = fxns.conversion;
1727
1728         % Selectivity 1 & 2
1729         hold on
1730         figure;
1731         tit = "Selectivity 1";
1732         xlab = "\chi";
1733         ylab = "S_1";
1734         plot(x, fxns.select_1);
1735         title(tit);
1736         xlabel(xlab);
1737         ylabel(ylab);
1738         hold off
1739
1740         hold on
1741         figure;
1742         tit = "Selectivity 2";
1743         xlab = "\chi";
1744         ylab = "S_2";
1745         plot(x, fxns.select_2);
1746         title(tit);
1747         xlabel(xlab);
1748         ylabel(ylab);
1749         hold off
1750
1751         % Reactor Volume
1752         hold on
1753         figure;
1754         tit = "Reactor Volume";
1755         xlab = "\chi";
1756         ylab = "V_{Reactor} [ m^3 ]";
1757         plot(x, fxns.V_plant .* M3_PER_L);
1758         title(tit);
1759         xlabel(xlab);
1760         ylabel(ylab);
1761         hold off
1762
1763         % Fresh feed flow rate of raw materials
1764         hold on
1765         figure;
1766         tit = "Fresh Feed of of Raw Materials into the Reactor [ kta ]";
1767         xlab = "\chi";
1768         ylab = "F_{FreshFeedRawMaterials}";
1769         for i = 1 : 15
1770             fxns.freshFeedRawMaterials(i,1) = 0;
```

```matlab
1771        end
1772        plot(x, fxns.freshFeedRawMaterials);
1773        % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↵
P_OVERRIDE, STEAM_MR_OVERRIDE);
1774        title(tit);
1775        xlabel(xlab);
1776        ylabel(ylab);
1777        hold off
1778
1779        % Production Rate of all reaction products leaving the reactor
1780        hold on
1781        figure;
1782        tit = "Production Rate [ kta ]";
1783        xlab = "\chi";
1784        ylab = "Production Rate" ;
1785        plot(x, fxns.productionRateRxnProducts);
1786        legend("Hydrogen", "Methane", "Ethylene", "Propane", "Butane")
1787        % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↵
P_OVERRIDE, STEAM_MR_OVERRIDE);
1788        title(tit);
1789        xlabel(xlab);
1790        ylabel(ylab);
1791        hold off
1792
1793        % Recycle flow rate of LR
1794        hold on
1795        figure;
1796        tit = "Recycle flow rate of Ethane [ kta ]";
1797        xlab = "\chi";
1798        ylab = "R_{Ethane}" ;
1799        for i = 1 : 15
1800            fxns.recycle(i,1) = 0;
1801        end
1802        plot(x, fxns.recycle);
1803        % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↵
P_OVERRIDE, STEAM_MR_OVERRIDE);
1804        title(tit);
1805        xlabel(xlab);
1806        ylabel(ylab);
1807        hold off
1808
1809        % Total flow rate to reactor
1810        hold on
1811        figure;
1812        tit = "Total flow rate to reactor [ kta ]";
1813        xlab = "\chi";
1814        ylab = "F_{RxtrIn}" ;
1815        for i = 1 : 15
1816            fxns.F_rxtr_in_total(i,1) = 0;
1817        end
1818        plot(x, fxns.F_rxtr_in_total);
1819        % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↵
P_OVERRIDE, STEAM_MR_OVERRIDE);
1820        title(tit);
1821        xlabel(xlab);
1822        ylabel(ylab);
1823        hold off
1824
```

```matlab
1825       % Total flow rate to the separation system
1826       hold on
1827       figure;
1828       tit = "Total flow rate to the separation system [ kta ]";
1829       xlab = "\chi";
1830       ylab = "F_{separation system}" ;
1831       for i = 1 : 15
1832           fxns.F_sep(i,1) = 0;
1833       end
1834       plot(x, fxns.F_sep);
1835       % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↙
P_OVERRIDE, STEAM_MR_OVERRIDE);
1836       title(tit);
1837       xlabel(xlab);
1838       ylabel(ylab);
1839       hold off
1840
1841       % Mol fraction of each component entering the separation system
1842       hold on
1843       figure;
1844       tit = "Mol fraction of each component entering the separation system [ kta ]";
1845       xlab = "\chi";
1846       ylab = "F_{i}" ;
1847       % for i = 1 : 15
1848       %    fxns.F_sep(i,:) = 0;
1849       % end
1850       plot(x, [fxns.x_hydrogen_sep, fxns.x_methane_sep, fxns.x_ethylene_sep, fxns.↙
x_propane_sep, fxns.x_ethane_sep, fxns.x_water_sep]);
1851       legend("Hydrogen", "Methane", "Ethylene", "Propane", "Butane", "Ethane",↙
"Water")
1852       % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↙
P_OVERRIDE, STEAM_MR_OVERRIDE);
1853       title(tit);
1854       xlabel(xlab);
1855       ylabel(ylab);
1856       hold off
1857
1858       % NPV
1859       hold on
1860       figure;
1861       tit = "NPV [ $ MM ]";
1862       xlab = "\chi";
1863       ylab = "NPV [ $ MM ]" ;
1864       tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↙
P_OVERRIDE, STEAM_MR_OVERRIDE);
1865       i = 1;
1866       fxns.npv(fxns.npv(:, 1) < 0, 1) = 0;
1867       fxns.npv(isnan(fxns.npv(:, 1)), 1) = 0;
1868
1869       % while (fxns.npv(i , : ) < 0)
1870          % fxns.npv(i, : ) = 0;
1871          % i = i + 1;
1872       % end
1873       plot(x, fxns.npv)
1874       % legend("Hydrogen", "Methane", "Ethylene", "Propane", "Butane", "Ethane",↙
"Water")
1875       title(tit);
1876       xlabel(xlab);
```

```matlab
1877        ylabel(ylab);
1878        hold off
1879
1880
1881
1882        % NPV (T, P, MR) | Varying T
1883 %    hold on
1884 %    figure;
1885 %    tit = "NPV [ $ MM ]";
1886 %    xlab = "\chi";
1887 %    ylab = "NPV [ $ MM ]" ;
1888 %    tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↙
P_OVERRIDE, STEAM_MR_OVERRIDE);
1889 %
1890 %    y = [];
1891 %    for i = 1:length(fxns.npv_T_P_MR(: , 1, 1 ))
1892 %        temp =fxns.npv_T_P_MR( i , 1, 1) ;
1893 %        y = [ y , fxns.npv_T_P_MR( i , 1, 1) ];
1894 %    end
1895 %
1896 % %    % Choose a colormap
1897 % %    cmap = jet(size(y, 2)); % Using 'jet' colormap; adjust the number of colors↙
based on the number of columns in y
1898 % %
1899 % %    for i = 1:size(y, 2) % Iterate through each column (dataset) in y
1900 % % %      temp =
1901 % %        plot(x, cell2mat(y(:,i)), 'Color', cmap(i,:), 'LineWidth', 2);
1902 % %    end
1903 %
1904 %    plot(x, y)
1905 %    title(tit);
1906 %    xlabel(xlab);
1907 %    ylabel(ylab);
1908 %    hold off
1909
1910
1911        % Sep cost vs conversion
1912        hold on
1913        figure;
1914        tit = "Separation Cost [ $ MM ]";
1915        xlab = "\chi";
1916        ylab = "Cost [ $ MM ]" ;
1917        % tit = tit + " " + sprintf("(%3.0f C %3.1f Bar %0.2f Steam MR)", T_OVERRIDE,↙
P_OVERRIDE, STEAM_MR_OVERRIDE);
1918        % i = 1;
1919        % fxns.npv(fxns.npv(:, 1) < 0, 1) = 0;
1920        % fxns.npv(isnan(fxns.npv(:, 1)), 1) = 0;
1921
1922        % while (fxns.npv(i , : ) < 0)
1923        %   fxns.npv(i, : ) = 0;
1924        %   i = i + 1;
1925        % end
1926        fxns.separationCosts(fxns.separationCosts(:, 1) > 10^9, 1) = 0;
1927        plot(x, fxns.separationCosts)
1928        % legend("Hydrogen", "Methane", "Ethylene", "Propane", "Butane", "Ethane",↙
"Water")
1929        title(tit);
1930        xlabel(xlab);
```

```
1931      ylabel(ylab);
1932      hold off
1933
1934
1935      % Return
1936      void = NaN;
1937 end
1938
```

I Team Member Work Statement

Team Member Work Statement

Name of team member here

Thejas Ravish

State here what you contributed to the design project and report

Hysys Models, writing of report, generation of tables/models for report

Name of team member here

Wesley Johnson

State here what you contributed to the design project and report

The entire codebase, all of the plots & figures. Lead team on all numerical simulation.

Name of team member here

Isaiah Huma

State here what you contributed to the design project and report

Level 2 & 3 mole balances, Hysys Models, Appendices, LaTex formatting, HAZOP, Generating Plots and tables in report, costing unit ops

Print Name and Sign: _Thejas Baishu_ Date: _3/13/24_

Print Name and Sign _[signature]_ Date: _3/13/2024_

Print Name and Sign _Isaiah Huma_ Date: _3/13/24_
[signature]

Rating of Team Members for Design Project

Please rate each group member's contributions in the categories below:
1-2 - unsatisfactory, 3 - acceptable/adequate, 4 – very good, 5 - excellent
Each member fills out one form and signs the bottom.

Name :	1) TJ	2) Isaiah	3) Wes
Quality of work presented	5	5	5
Quantity of work performed	5	5	5
Effort	5	5	5
Punctuality (meetings and deadlines)	5	5	5
Knowledge of design methods	4	5	5
Class attendance	5	5	5

Communication _____ 5   _____ 5   _____ 5

Do you feel that each member of the group deserves the same grade? If not, who does not and why?

Yes

It's important to note that differences in performance will not necessarily affect individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

Print Name and Sign: __Thejas Ravish_____ Date: __3/13/23__