Ethylene Production by Thermal Steam Cracking of Ethane

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Group 1

Executive Summary

This report contains a detailed techno-economic analysis describing a profitable and carbon-neutral steam ethane cracker with an ethylene production rate of 200 kta up to Level 5 of the Douglas hierarchy of plant design. The scope of this plant analysis includes a distillation system, isothermal-isobaric reactor, along with a heat exchanger network with furnaces and coolers. The proposed plant is designed to sell 200 kta of polymer-grade ethylene at $900/MT produced from an ethane feed of 270 kta purchased at $200/MT. If a pressure swing adsorption (PSA) separation system is added to the plant, chemically pure hydrogen can be sold as a coproduct at $1400/MT. We determined that the optimal reactor conditions include a volume of 16 m^3 with a height to length ratio of 10:1, an operating temperature of 825 C, an operating pressure of 2 bar, and an inlet steam-to-ethane molar ratio of 0.6 for the plug flow reactor (PFR). Kinetic modeling in MATLAB and an Aspen Hysys simulation predict an ethane conversion of 73% in the PFR at these conditions. Coproducts propane, butane, and methane are separated and sold for their fuel value at $3/GJ. Unreacted ethane is separated and recycled to the reactor inlet. Fresh ethane and steam is fed to the plant at 30600 kg/hr and 14000 kg/hr, respectively. Additionally, 0.5 kg of CO_2 is produced per 1 kg ethylene produced. At this level we predict an energy requirement of 14 MJ per kg of ethylene product. The cracker and associated equipment assumes a 15-year operational lifespan and 3 year construction period. Reactor and separation conditions and dimensions were optimized with respect to the maximum net present value of the unit (NPV). For a preliminary design including PSA, the overall optimized economic analysis yields an NPV, TCI, and IRR of $124 MM, $112 MM, 32%, respectively. The NPV before tax returns indicate profitability in this sector. Sensitivity analysis demonstrates a large range of economic fluctuations that allow this plant to have a positive NPV.

Process Flow Diagram — stream and equipment labels:

Feed streams
- 1 — 33870 kg/h, 25 C, 2 bar
- 2 — 34500 kg/h, 121 C, 2 bar

HEX 1 — 125000 GJ/h, UA ~ 1.7e6
- 3 — 58500 kg/h, 84 C, 2 bar
- 4 — 58500 kg/h, 759 C, 2 bar

Heater 1 — 13480 GJ/h, 1.8 MW
- 5 — 58500 kg/h, 825 C, 2 bar

Reactor 1 — 128300 GJ/h, Conversion 72%
- 6 — 58500 kg/h, 825 C, 2 bar
- 7 — 58500 kg/h, 167 C, 2 bar

HEX 2 — 7213 GJ/h, UA ~ 1.2e6
- 8 — 58500 kg/h, 136 C, 2 bar
- 9 — 58500 kg/h, 80 C, 2 bar

Cooler 1 — 41880 GJ/h, 12 MW
- 10 — 5 C, 2 bar
- 11 — 14320 kg/h, 5 C, 2 bar

Flash 1
- 12 — 44170 kg/h, 5 C, 2 bar

PSA 1 — 4 Columns
- 13 — 44000 kg/h, 8.6 C, 2 bar
- 14 — 170 kg/h, 120.2 C, 2 bar

Cooler 2 — 29990 GJ/h, 8.3 MW
- 15 — 44000 kg/h, -35 C, 2 bar

Flash 2
- 16 — 44000 kg/h, -140 C, 2 bar

HEX 4 — 4059 GJ/h, UA ~ 4e4
- 17 — 44000 kg/h, -140 C, 2 bar
- 18 — 2630 kg/h, -140 C, 2 bar

Compressor 1 — 3641 GJ/h, 1 MW
Heater 2 — 13480 GJ/h, 1.8 MW
- 19 — 2630 kg/h, -30.5 C, 13 bar

PSA 2 — 4 Columns
- 20
- 21 — 1742 kg/h, 0 C, 2 bar
- 22 — 2639 kg/h, 25 C, 13 bar / 886.6 kg/h, 116 C, 2 bar

- 23 — 41360 kg/h, -96 C, 2 bar

Pump — 580 GJ/h, .2 MW
- 24 — 41360 kg/h, -92 C

Heater 3 — 13480 GJ/h, 1.8 MW
- 25 — 41360 kg/h, -62 C, 60 bar
- 26 — 41360 kg/h, -0.3 C, 60 bar

HEX 5 — 7464 GJ/h, UA ~ 3.5e4
- 40 — 14320 kg/h, 1.1 C, 2 bar

HEX 3 — 7800 GJ/h, UA ~ 2e5
- 39 — 14320 kg/h, 117 C, 2 bar

- 27 — 41360 kg/h, 34.6 C, 60 bar
- 28 — 41360 kg/h, 32.29 C, 60 bar

Expander 1 — 1272 GJ/h, -0.3 MW

Cooler 3 — 9148 GJ/h, 2.6 MW
- 29 — 41360 kg/h, -24 C, 16 bar
- 30 — 41360 kg/h, -30.63 C, 16 bar
- 31 — 41360 kg/h, -30.63 C, 16 bar

Distillation Column 1 — 60 Stages, Feed: Stage 37, R = 3.95
Condenser 1 — 46510 GJ/h, 13 MW
Reboiler 1 — 46740 GJ/h, 13 MW
- 32 — 23090 kg/h, -33.5 C, 10 bar
- 33 — 54.6 kg/h, -75 C, 10 bar
- 34 — 17620 kg/h, -8 C, 16 bar

Distillation Column 2 — 14 Stages, Feed: Stage 4, R = 1.41
Condenser 2 — 3 MW
Reboiler 2 — 11640 GJ/h, 1.2 MW
- 35 — 12130 kg/h, -17 C, 16 bar
- 36 — 5485 kg/h, 93.1 C, 16 bar

HEX 6 — 1652 GJ/h, UA ~ 4e4
- 37 — 12130 kg/h, -17 C, 16 bar

Expander 2 — 397 GJ/h, 0.1 MW
- 38 — 12130 kg/h, -75.5 C, 2 bar

Stream Name	1	2	3	4	5	6	7	8	9	10
Vapor Fraction	1.00	1.00	0.90	1.00	1.00	1.00	1.00	1.00	0.98	0.75
Temperature [C]	25.00	121.00	84.63	759.42	825.00	825.00	166.97	115.96	80.13	5.00
Pressure [kPa]	200.00	200.00	200.00	200.00	200.00	200.00	200.00	200.00	200.00	200.00
Molar Flow [kgmole/h]	1060.00	805.00	2269.06	2269.06	2269.06	3137.36	3137.36	3137.36	3137.36	3137.36
Mass Flow [kilo tonne/year]	279.41	127.13	512.79	512.79	512.79	512.79	512.79	512.79	512.79	512.79
Comp Mole Frac (Ethylene)	0.00	0.00	0.01	0.01	0.01	0.28	0.28	0.28	0.28	0.28
Comp Mole Frac (Ethane)	1.00	0.00	0.64	0.64	0.64	0.13	0.13	0.13	0.13	0.13
Comp Mole Frac (Methane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (Hydrogen)	0.00	0.00	0.00	0.00	0.00	0.31	0.31	0.31	0.31	0.31
Comp Mole Frac (Propane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (n-Butane)	0.00	0.00	0.00	0.00	0.00	0.03	0.03	0.03	0.03	0.03
Comp Mole Frac (H2O)	0.00	1.00	0.35	0.35	0.35	0.26	0.26	0.26	0.26	0.26

Stream Name	11	12	13	14	15	16	17	18	19
Vapor Fraction	0.00	1.00	1.00	0.00	1.00	0.42	0.00	1.00	1.00
Temperature [C]	5.00	5.00	8.81	120.23	-35.51	-140.00	-140.00	-140.00	-10.51
Pressure [kPa]	200.00	200.00	200.00	200.00	200.00	200.00	200.00	200.00	1300.00
Molar Flow [kgmole/h]	795.08	2342.28	2332.36	9.92	2332.36	2332.36	1347.29	985.07	985.07
Mass Flow [kilo tonne/year]	125.56	387.23	385.66	1.57	385.66	385.66	362.53	23.13	23.13
Comp Mole Frac (Ethylene)	0.00	0.38	0.38	0.00	0.38	0.38	0.64	0.02	0.02
Comp Mole Frac (Ethane)	0.00	0.17	0.17	0.00	0.17	0.17	0.29	0.00	0.00
Comp Mole Frac (Methane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (Hydrogen)	0.00	0.41	0.41	0.00	0.41	0.41	0.00	0.97	0.97
Comp Mole Frac (Propane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (n-Butane)	0.00	0.04	0.04	0.00	0.04	0.04	0.07	0.00	0.00
Comp Mole Frac (H2O)	1.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00

Stream Name	21	22	23	24	25	26	27	28	29	30
Vapor Fraction	1.00	1.00	0.00	0.00	0.00	0.00	1.00	1.00	0.65	0.00
Temperature [C]	0.00	-115.98	-96.00	-92.45	-62.45	0.33	34.58	32.29	-24.13	-30.63
Pressure [kPa]	200.00	200.00	200.00	6000.00	6000.00	6000.00	6000.00	6000.00	1600.00	1600.00
Molar Flow [kgmole/h]	864.16	120.91	1347.29	1347.29	1347.29	1347.29	1347.29	1347.29	1347.29	1347.29
Mass Flow [kilo tonne/year]	15.27	7.86	362.53	362.53	362.53	362.53	362.53	362.53	362.53	362.53
Comp Mole Frac	0.00	0.18	0.64	0.64	0.64	0.64	0.64	0.64	0.64	0.64

(Ethylene)									
Comp Mole Frac (Ethane)	0.00	0.02	0.29	0.29	0.29	0.29	0.29	0.29	0.29	0.29
Comp Mole Frac (Methane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (Hydrogen)	1.00	0.79	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (Propane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (n-Butane)	0.00	0.00	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07
Comp Mole Frac (H2O)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Stream Name	32	33	34	35	36	37	38	39	40
Vapor Fraction	0.00	1.00	0.00	0.00	0.00	0.23	0.46	0.00	0.00
Temperature [C]	-38.52	-38.52	-8.10	-17.27	93.06	-17.15	-75.52	117.90	1.07
Pressure [kPa]	1600.00	1600.00	1600.00	1600.00	1600.00	1600.00	200.00	200.00	200.00
Molar Flow [kgmole/h]	844.77	2.00	500.52	404.37	96.15	404.37	404.06	795.08	795.08
Mass Flow [kilo tonne/year]	207.63	0.48	154.42	106.34	48.08	106.34	106.25	125.56	125.56
Comp Mole Frac (Ethylene)	1.00	0.97	0.03	0.04	0.00	0.04	0.04	0.00	0.00
Comp Mole Frac (Ethane)	0.00	0.00	0.79	0.96	0.04	0.96	0.96	0.00	0.00
Comp Mole Frac (Methane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (Hydrogen)	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (Propane)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Comp Mole Frac (n-Butane)	0.00	0.00	0.18	0.00	0.96	0.00	0.00	0.00	0.00
Comp Mole	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00	1.00

Frac (H2O)									

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1 Introduction

1.1 Motivation and Background

Analysts at BICC have determined the demand for polymer-grade ethylene will exceed supply by ~2000 kta, which would allow BICC to secure market share by producing 200 kta of ethylene[1]. The proposed process in development will sell the product ethylene at \$900/MT with the option to sell co-product Hydrogen at \$1400/MT. Preliminary economic analysis has demonstrated the maximum economic potential for an ethane steam cracker with a PSA to be ~\$157MM/year[2]. Moreover, by sequestering CO_2 at a cost of \$125/MT, we address environmental concerns and align with BICC's sustainability goals[1]. We are motivated to quickly enter the polymer-grade ethylene market based on the opportunity to secure an ethane source contract at \$200/MT[1].

1.2 Market Analysis

Our team has conducted a comprehensive market analysis for BICC Inc.'s proposed ethylene production plant. This analysis incorporates findings from recent industry reports, projecting a notable surge in global ethylene demand. As of 2021, the global ethylene market volume reached approximately 150,000 kta, with forecasts predicting a growth at a compounded annual growth rate (CAGR) of 4.09% to 2035[7]. This upward trend provides BICC with a window to capitalize on the anticipated market expansion and the existing supply-demand gap with ethylene.

Previous market research highlights that ethylene demand is set to outstrip supply by at least 2,000 kta within the next 2 years[1]. An example of recent demand increases on chemical plant success is demonstrated by Lotte Chemical's investment in a mega petrochemical plant in Indonesia, utilizing naphtha cracking technology with an estimated ethylene production rate of 1,000 kta[7]. This venture alone is expected to generate 2.06 billion USD annually upon its completion in 2025 emphasizing the lucrative nature of the ethylene market[7]. The market dynamics are further shaped by ethylene's major application in polyethylene production, in which 54% of ethylene production was used in the polyethylene industry in 2021[18].

The hydrogen market was explored because it is a potential supplementary revenue source for the proposed ethylene production plant, leveraging a PSA system utilizing a bed composed of zeolite 5A. This exploration revealed that hydrogen sales could enhance the project's success. Analysis of the global hydrogen market anticipates growth, driven by expansions in chemical synthesis, fuel, and energy storage sectors[8]. Concurrently, variations in ethylene and hydrogen pricing, alongside investments in low-carbon and renewable hydrogen production, are reshaping the market.

1.3 Reaction Chemistry

This set of three reactions shown below is an accurate description of the reaction kinetics within the conditions of 775-825°C and 2-5 bar. The reaction rate of reaction 1 is approximately

an order of magnitude greater than reaction 3, while reaction 2 is 5 orders of magnitude slower than reaction 1.

$$C_2H_6 \rightleftharpoons C_2H_4 + H_2 \tag{1}$$

$$2C_2H_6 \rightarrow C_3H_8 + CH_4 \tag{2}$$

$$C_2H_6 + C_2H_4 \rightarrow C_4H_{10} \tag{3}$$
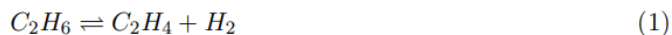
Reaction 1 is highly endothermic with a reaction enthalpy of 1.4×10^5 J/mol. Reactions 2 and 3 are exothermic with reaction enthalpies of -4.73×10^3 and -9.4×10^4 J/mol. The overall reaction set is endothermic because of the highly endothermic nature of the fastest reaction. The kinetic models, rate expressions, and temperature dependence are explicitly outlined in Appendix C.

2 Conceptual Design

2.1 Process Overview & Simulation

The proposed process includes design decisions up to level 5 of the Douglas hierarchy of plant design[1]. The level 1 decision was to employ an ethane cracker for the production of ethylene. This decision was made by BICC via a comprehensive historical data, economic viability, and the availability of ethane[1]. At level 2 we decide to completely recycle unreacted ethane from the reactor effluent. At level 3 we decide to use an isothermal-isobaric ideal plug flow reactor (PFR) and perfect separation system. Mole balances are derived in detail for the proposed design up to level 3 in detail in Appendix D. We first model the conceptual design of the PFR using MATLAB to optimize key reactor design variables: temperature, pressure, steam-to-ethane molar ratio, and volume relative to economic parameters. The MATLAB simulation is then verified using an Aspen Hysys simulation and matches our conceptual design within ~1% of key process parameters and metrics. After verification, we opted to sell coproducts methane, propane, and butane based on their combustion heat value rather than recycling them as fuel. Level 4 includes the designs for a more realistic separation system including distillation towers and flash drums. At level 5 we determine an integrated energy balance and heat exchange network to address costs associated with outsourced heating (burning methane) and cooling (purchasing refrigerant) that can be solved inside the plant. The design decisions for Level 1-3 are shown in Figure 1, a comprehensive process flow diagram is shown on page 2. Design decisions for the heat exchanger network and separation system are shown on Appendix D and are explicitly illustrated on page 2.
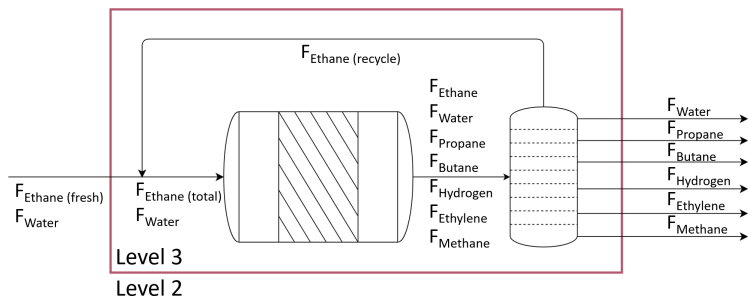
Figure 1. Level 2 and Level 3 decisions for the proposed steam-ethane cracker

2.1.1 Key Design Parameters

In this stage of process development we are able to vary reactor temperature, reactor volume, steam-to-ethane ratio, pressure, and the optional use of a PSA. We determine these optimal parameters by systematically varying different reactor volumes within our MATLAB simulation and maximizing economic parameters. One furnace and heat exchanger is used to heat the incoming streams before it enters the pyrolysis furnace containing the PFR. The separation system consists of two flash drums, two distillation columns, and two PSA systems. There are a total of 17 heat exchangers within the plant and 2 compressors and 2 expanders. The pressure at which we distill ethylene to desired purity, and then subsequently ethane for recycle has a large effect on the profitability of the plant and is considered after the reactor has been optimized. The operating pressure of the distillation in this design is determined systematically in HYSYS by varying the pressure and observing the trend in NPV.

BICC's decision to operate a carbon neutral ethylene plant is also extremely important in our overall design. Although it limits potential profit of the company, it is important to ensure profitability while paying for CO_2 sequestration as future legislation and current tax rates within the lifetime of the plant may require it. Ensuring plant profitability at this level therefore protects potential future profits and aligns with our sustainability goals as a company.

2.3 MATLAB PFR Simulation & Optimization

2.3.1 PFR Simulation

An ideal isothermal-isobaric PFR is modeled in MATLAB by using the PFR algorithm outlined in Digital Design of Chemical Processes[9]. The outlet flows at specific reactor volumes are shown in Figure 2A as a result of the simulation. From this simulation we can extract the selectivity vs. conversion for this set of reactions at various temperatures, with a constant pressure and steam-to-ethane ratio shown in Figure 2C. A fully comprehensive compilation of these design variable variations is shown in Appendix A.
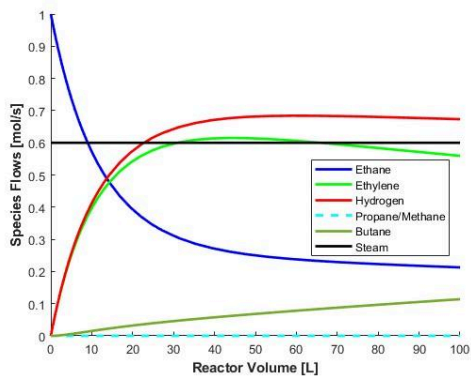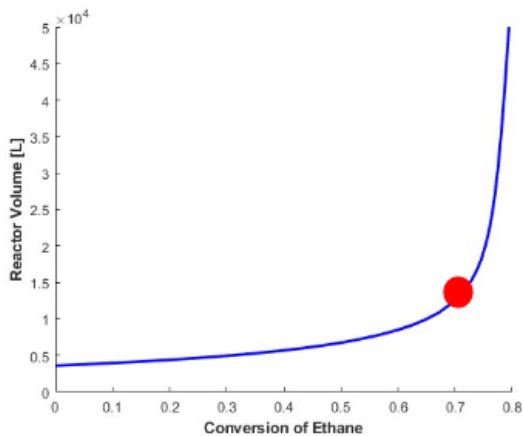
2A.
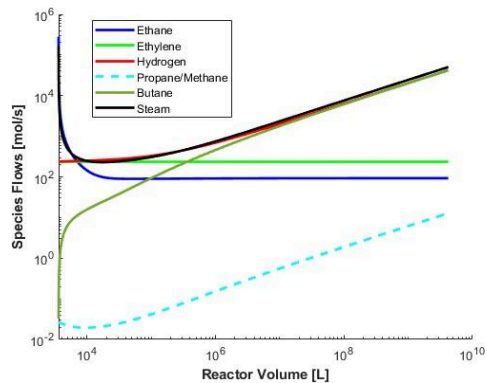
2B.
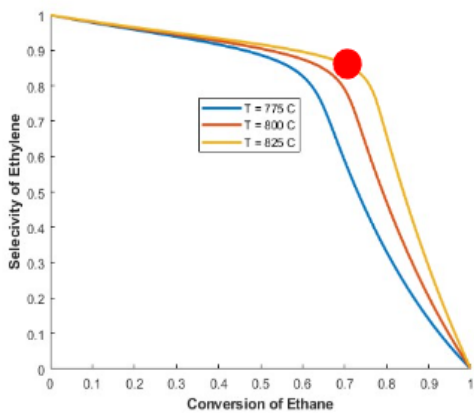
2C.

2D.

Figure 2. 2A. Reactor effluent species flows (mol/s) down the volume of the PFR with operating conditions of T= 825°C, P = 2bar, and steam-to-ethane molar ratio of 0.6 entering the reactor (1 mol/s basis)

2B. Scaled Reactor effluent species flows at different reactor volumes with a fixed production rate of 200kta of ethylene at T= 825°C, P = 2bar, and steam-to-ethane molar ratio of 0.6.

2C. Selectivity of ethylene vs. conversion of ethane at different operating temperatures and a fixed operating pressure of 2 bar. As the temperature increases the selectivity of ethylene/ethane increases.

2D. Reactor volume [L] vs. conversion of ethane. A finite volume is required at 0 conversion due to the specified production rate of ethylene (200kta).

Species flows and reactor volume shown in Figure 2A need to be scaled to reach the specified production rate of 200kta of ethylene. Effluent species flow is scaled via the PFR algorithm and is shown in Figure 2B. The general trend of reactor volume vs. conversion is shown in Figure 2D. From Figure 2C-D we see a sharp decrease in selectivity and a large increase in reactor volume, indicating that the optimal conversion is likely between 0.65 and 0.75.

A comprehensive process flow diagram is shown on page 2. Fresh feed ethane enters the process at 1060 kgmol/hr as a pressurized liquid at 25 C and is mixed with 805 kgmol/hr steam at 121 C and 2 bar and is heated to reach a temperature and pressure of 825C and 2 bar. This

stream is then mixed with 404 kgmol/hr of pure recycled ethane at -75.5C and 2 bar prior to entering the reactor. The reactor inlet has a steam-to-ethane molar ratio of 0.6. The PFR is operated isothermally to insure an operating temperature of 825ºC and we assume no pressure drop across the reactor to model it as isobaric. The reactor effluent is then separated to produce streams of hydrogen, methane, ethane, ethylene, propane, and butane. At this level of reactor optimization we assume all ethane is recycled. Ethylene is sold as a cooled and pressurized liquid and methane and butane are sold at fuel value. At this stage of process development we have moved forward with including a PSA system to purify 90 mol% of the outlet hydrogen stream so that we can sell chemically pure hydrogen. The remaining 10 mol% of the effluent hydrogen is used as the sweep gas to remove methane and ensure chemical purity of the hydrogen stream is reached. We run net present value optimization in the following section to determine if this is the most economical choice of reactor conditions.

### 2.3.2 Net Present Value Reactor Optimization at Level 3

Optimal values for key design parameters must be found via economic analysis and optimization. Specifically, reactor temperature, pressure, volume, and steam-to-ethane are optimized with respect to net present value (NPV) of the plant at the end of the 18 year project lifetime (3 years of construction and 15 years of operation) and the use of a PSA is considered. The optimal PFR conditions include an operating temperature of 825 C, reaction pressure of 2 bar, steam-to-ethane molar ratio of 0.6, and a volume of 16 m^3 (corresponding to a single pass ethane conversion of 0.73) along with the use of a PSA. The optimal NPV corresponding to these reactor conditions is ~$140 MM with a PSA and is determined by Figure 3A. The optimal NPV with the same reactor conditions and no PSA is ~$100 MM. General trends of the effect of reactor temperature, pressure, volume, and steam-to-ethane molar ratio on a reactor with a PSA are shown in Figure 3B-D. Similar trends are shown for the no PSA system in Figure A6-9.
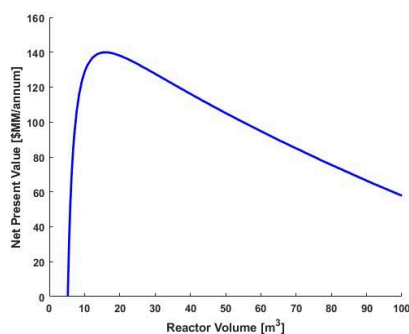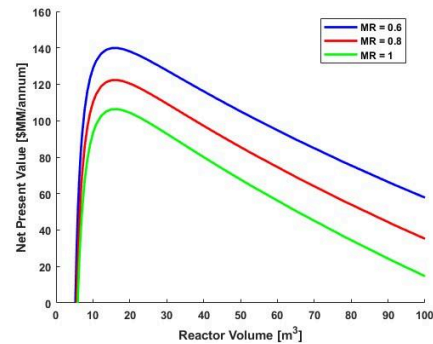

3A.
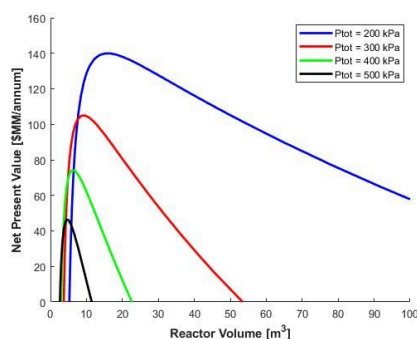
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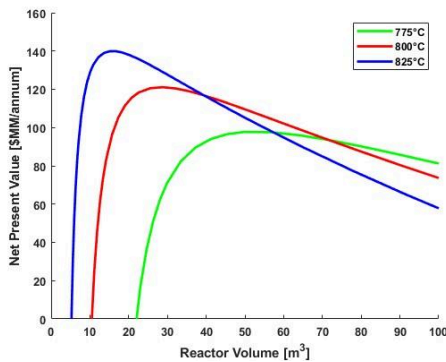
3C.	3D.

Figure 3. 3A. NPV[$MM] vs. reactor volume [L] for a PFR including a PSA with an operating pressure of 2 bar and temperature of 825 C and steam-to-ethane molar ratio of 0.6.

3B. NPV[$MM] vs. reactor volume [L] for a PFR including a PSA with a varying operating pressure of 2 -5 bar and at a temperature of 825 C and steam-to-ethane molar ratio of 0.6.

3C. NPV[$MM] vs. reactor volume [L] for a PFR including a PSA with a varying operating temperature of 775-825C at an operating pressure of 2 bar and steam-to-ethane molar ratio of 0.6.

3D. NPV[$MM] vs. reactor volume [L] for a PFR including a PSAwith a varying steam-to-ethane molar ratio of 0.6 to 1 at a temperature of 825 C and operating pressure of 2 bar.

We observe that at higher temperature, lower pressure, and lower steam-to-ethane molar ratio the NPV increases, due to Le Chatliers principle which increases the selectivity at these conditions. As the operating pressure of the PFR increases from 2 bar to 5 bar, the NPV decreases as shown in f 3B. As the operating temperature of the PFR increases from 775 C to 825 C the NPV increases as shown in Figure 3C. Increasing the steam-to-ethane molar ratio from 0.6 to 1 decreases the NPV as shown in Figure 3D. The MATLAB script used to calculate the maximum NPV and other relationships is in Appendix I.

We considered the cost of steam, ethane, CO_2 sequestration taxes, furnaces, the PFR, and a simplified separation system when optimizing for NPV. Costing of each of these parameters is described explicitly with their associated cost correlations in Appendix F and optimal reactor parameters are valued in Section 3. We decided to not recycle produced propane and butane to heat the plant because purchasing natural gas has a better generated energy per generated CO_2 ratio indicating that it is more economical to buy natural gas to heat the plant. The use of a hydrogen PSA system requires a bed of zeolite 5A which has negligible cost compared to other economic parameters as shown in the costing correlation in Appendix E.6. The PSA tank itself is costed as a pressure vessel shown in Appendix E.1.3. NPV optimization is heavily dependent on the energy required to heat inlet streams and separate reactor outlet streams.

The following subsections utilize this PFR and conditions to create a detailed design of the separation system and heat exchanger network as part of Level 4 and 5 of Douglas's hierarchy of design. Further optimization of reactor design via MATLAB is not considered due to the reliance on HYSYS for a detailed separation system design.

2.3.3 Separation System Design & Optimization (Level 4)

The separation system consists of 2 flash drums, 2 PSA systems, and 2 distillation columns. The flash drum capital expenses are relatively small compared to the total capital expenses; only the coolant required to liquify the entering stream was varied to optimize NPV. The first flash drum is used to remove most of the steam exiting the reactor as a water stream at 5 C. The trace water that remains in the product stream is removed using the first PSA. 5 C was chosen as the flashing temperature because this allows for most of the water to be removed without freezing water within the system. The second flash drum is used to remove most of the hydrogen from the product stream at -140 C.

The recovered hydrogen stream is sent through a hydrogen PSA which recovers 90 mol% of the incoming hydrogen stream and uses 10 mol % as sweep gas to remove the ethylene, ethane, and methane adsorbed to the zeolite within the beds. The capital expenses of the PSA consist of ~3200 kg of zeolite 5A with 80% loading and four pressure vessels sized to allow for 99.999 wt % of hydrogen gas to be purified. The PSA design algorithm, assumptions, and piping and instrumentation diagram is shown in Appendix E.6.

The effluent from the first flash drum is sent through a water PSA to remove trace water from the system to prevent freezing further downstream. The water PSA is costed based on the minimum thermodynamic work requirement to separate the remaining water from the stream and scaled by 35 as an energy efficiency factor. Capital and operating expenses are determined based on the scaled minimum thermodynamic work, similar to the estimated expenses used for the separation system from the reactor optimization in section 2.3.2 and outlined in Appendix E.2.

A distillation column is used to separate ethylene from butane and ethane, then another is used to separate the ethane from the ethane/butane stream to allow for ethane + trace ethylene recycling. The first distillation column parameters (# of trays, reboil ratio, reflux ratio, feed stage location) were determined based on the required purity of ethylene (99.9 mol%) via the Fenske-Underwood-Gilliland (FUG) method outlined in Appendix C.2 and uses relative volatility plots shown in Appendix J. This method assumes constant relative volatility and is based on the Gilland correlation, indicating that further optimization of distillation column parameters is required via HYSYS to produce the desired purity of the product. The second distillation tower size was similarly estimated and further optimized in HYSYS. The column parameters vary depending on the distillation pressure and are described for the highest NPV design following Table 1. Finally, the distilled Ethane is 99.1% recycled which yields a plant conversion very close to 1, where only 110 kg/hr of ethane is sold with butane as fuel compared to a feed of ~32,000 kg/hr of ethane.

The largest effect on NPV of the distillation columns comes from the operating expenses of the refrigeration for the condenser and the power to reboiler. Capital expenses for the reboilers, condensers, flash drums, and distillation columns are small (~ $10 MM) compared to the refrigeration operating expenses (~ $54 MM/year) so the energy requirements of the condensers and coolers were mainly used to optimize NPV at this stage of plant design.

We varied the pressure within the distillation columns at 2 bar, 16 bar, and 22 bar to determine the optimal pressure within the column. The separation becomes less effective and more energy intensive at higher pressures, however, the cost of refrigeration decreases exponentially[19] with temperature, indicating need for optimization. We determined different NPVs for different separation pressures of 16 bar, 22 bar, and 2 bar with values shown in Table 1. The highest NPV of $ 124.4 MM corresponded to a separation pressure of 16 bar.

Distillation Pressure [bar]	NPV [$MM]
2	88.5
16	**124.4**
22	118.2

Table 1. NPV versus pressure within the distillation columns

The highest NPV design at 16 bar for the first distillation column has 60 trays, a reboil ratio of 8.2, a reflux ratio of 4.5, and the feed tray is located at stage 37 (top down numbering) and produces a product purity of 99.92 mol% ethylene with trace hydrogen and ethane. The highest NPV design at 16 bar for the second distillation column has 14 stages, a reboil ratio of 6.7, a reflux ratio of 1.41, and the feed tray is located at stage 4 (top down numbering). These towers are fed 1347 kgmol/hr and 500 kgmol/hr of material, respectively.

2.4 Energy Integration and Balances (Level 5)

We used heat integration via a heat exchanger network to reduce the heat and cooling costs associated with our proposed process. Level 3 conceptual designs estimate a total energy expenditure of 123MW through the plant. With our inclusion of 6 heat exchangers that exchange heat between process streams, our energy usage at level 5 is 92 MW. From our heat integration we save 31 MW of heating or cooling.
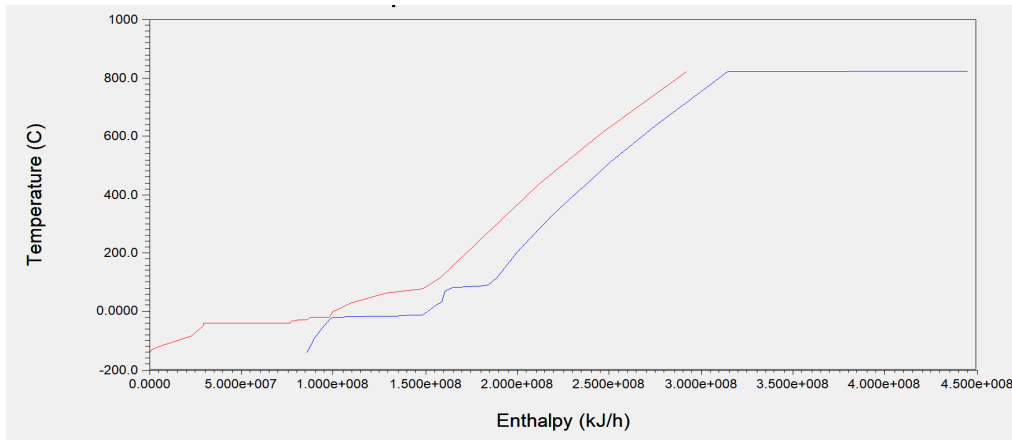

Figure 4: A composite heat map of our overall plant design.

Based on the composite heat map shown in Figure 4, we determined heat exchanger locations by using a pinch analysis provided by the HYSYS Energy Analysis tool to give optimal heat exchanger sizes and locations. This process in conjunction with intuitive placement yields 6

heat exchangers which reduce energy expenditure by ~31 MW across the plant. The maximum ΔT within the heat exchangers was 120 C to reduce thermal stress within the stream exchangers and the maximum trim ΔT was set to 10 C. Within reboilers the ΔT was below 50 C to prevent film boiling. Heat exchanger sizing and costing is shown in Appendix E.4 and the connections between heat exchangers and process streams is shown explicitly on page 2.

2.4.1 Coolers

We have three coolers used to cool process streams, each treated as heat exchangers, and are each cooled with external streams of refrigerant bought as a utility. Our first cooler is a series of three heat exchangers before our first water flash drum. We are cooling the reactor effluent from 80 C to 5 C using 3 heat exchangers each with an area of 25,000 ft². We used the duty calculated from Hysys and the equation,

$$Q \;=\; n \cdot A \cdot U \cdot \Delta T$$

In which Q is the duty to cool [W], n is the number of heat exchangers we need to use if the total calculated area exceeds 25,000 ft², to which our correlation applies. A represents the area of the heat exchanger [m²], U is the heat transfer coefficient [W/m²K], and ΔT is the log mean temperature difference [K]. We purchase our refrigerant 10 C cooler than the temperature we need to achieve, ensuring there is at least a 10 C difference for trim. This prevents oversized heat exchangers. Our second cooler in the plant cools the dry process stream from -35°C to -140°C to flash the hydrogen out, with an exchanger with 16,500 ft² of area. This process is one of the most expensive in the plant due to the refrigerant. For this cold stream, we determined that it would be more expensive to buy refrigerant 10 degrees cooler than -140°C, than to build a larger heat exchanger. For this stream alone, we purchased refrigerant at -141°C and used a larger heat exchanger. The last cooler is used before the first distillation column to ensure that the stream is a saturated liquid. This cooler lowers the process stream from -24°C to -30°C. We bought refrigerant 10 degrees cooler than the -30°C needed to cool the stream, to keep the heat exchanger with an area of 9930 ft².

2.4.2 Heaters

Energy requirements for the unit are met by burning natural gas and paying a carbon sequestration tax. For simplicity, we assume that natural gas is 100% methane. To produce one kg of ethylene, we use approximately 14 MJ of energy. This is equivalent to 0.5 kg of CO2 produced per kg of ethylene and requires 0.2 kg of natural gas. Therefore this plant produces 100 kta of CO_2 at this level of design. At this stage, we estimate that heating the feed streams to reactor inlet conditions and the separation system requires the majority of the energy consumed by this plant, with a total energy requirement of approximately 92 MW or ~ 2.8 PJ/year. We assume no pressure drop through the plant/unit operations or heat loss to the surroundings at this stage.

We require three furnaces in the proposed process. One pyrolysis furnace is required to heat the PFR because the overall steam ethane cracking reaction is endothermic. A process

furnace is needed to heat the feed ethane, steam, and recycled ethane before entering the pyrolysis furnace. A second process furnace is used after the pump following the second (hydrogen) flash, which is heated to reduce the temperature difference to lower than 120 C before it enters a heat exchanger to be further heated by the water from the first flash. Refer to page 2 to see the full heat exchanger network and integration. The pyrolysis furnace requires approximately 36 MW, the first process furnace requires about 3.9 MW during standard operation, and the second process furnace requires about 0.8 MW during standard operation.

2.4.3 Separation System Energy Requirements

Through level 3 of the design process the separation system including a PSA system requires ~58 MW for operation. This value was estimated using the scaled minimum thermodynamic work required to separate components and is outlined in Appendix E.2. At level 5 of the design we use 2 distillation towers, 2 flashes, and 2 PSA's. The separation system requires 55MW. This value is 3 MW lower than the predicted energy requirement due to the heat exchanger network within the plant. The largest energy expenditure of the separation system is in the condenser and reboiler of the first distillation column with an energy expenditure of 26 MW. The second largest is the process cooler that brings the temperature down to -140 C for the hydrogen flash with an energy use of 8 MW. The second distillation tower requires 6 MW of energy for the reboiler and condenser. The energy requirement for the hydrogen PSA is 1 MW based on the compressor used to raise the pressure from 2.5 bar to 12.5 bar. The energy requirement for the water PSA system was approximated as 4.4 MW based on a scaled minimum thermodynamic work. Refer to Appendix E.2 for further details.

To reduce energy consumption, we pump the liquid product stream leaving the hydrogen flash to higher pressure. Liquid pumps require very little work (~0.1 MW) and therefore have a small operating expense. The high pressure liquid is then sent through a heat exchanger network and is eventually vaporized in a kettle reboiler heat exchanger which produces high pressure gas. The gas is subsequently expanded using an adiabatic expansion nozzle to drop the temperature significantly prior to being condensed to a saturated liquid to enter the first distillation column.

3 Economic Analysis

3.1 Equipment List

The proposed process development involves at least 4 main pieces of equipment, with the possible addition of a PSA system. Cost correlations used for the pieces of equipment in this report used the Marshall and Swift Index with a value of 1800 for the year of 2024[1]. As well, full calculations and cost correlations for equipment are shown in Appendix E.

The PFR is modeled and costed as a pressure vessel rated up to 50 psi with a volume of 16 m^3 and a length to diameter ratio of 10:1. It is constructed out of stainless steel rather than carbon steel (a potential cheaper option) because this plant is run at high temperatures for

prolonged periods of time and produces hydrogen which reacts with carbon at high temperatures within the metal walls.

The pyrolysis furnace which houses the PFR and the process furnace used to heat the inlet streams are constructed from a chromium/molybdenum alloy. This material is chosen because of its ability to resist reactions/corrosion and from its proven use in the oil and gas industry[11]. The process furnace is used to heat fresh ethane, steam, and recycle ethane is similarly constructed from a chromium/molybdenum alloy because of the potential requirement for corrosion resistance.

Distillation capital expenses (CAPEX) consisted of three parts: tray costing, pressure vessels, and the heat exchangers for the reboiler and the condenser. Out of these three parts, the most expensive was determined to be the heat exchangers, contributing to most of the cost for our distillation system. We use stainless steel for each material and the tower is assembled with sieve trays at 24 inch spacing. The system of two distillation columns accounts for ~$4MM of our inside battery limit (ISBL).

The heat exchangers across the plant for heat integration are all costed to maximize surface area, up to 25,000 ft^2 depending on their operation pressures and heat duty. Additionally, the tower reboilers were designed as kettle reboilers to allow for vapor volume whereas all stream heat exchangers are shell and tube design.

Flash drums across the plant are costed as pressure vessels constructed of stainless steel and were designed to flash at 2 bar but are rated to ~3.4 bar.

Equipment Name	Description	Material	Size[m^3]	Duty [MW]	CAPEX [MM$]
PFR	Pressure vessel at 10:1 length to diameter ratio	SS	16	~	0.3
Distillation Column 1	Ethylene/Ethane+Butane+Trace Splitter	SS	65 (60 stages)	26	3
Distillation Column 2	Ethane/Butane+Trace Splitter	SS	15 (14 stages)	6	1.1
Furnace 1	Pyrolysis furnace	Chrome/Mo Alloy	Outside Scope	36	0.6
Furnace 2	Process furnace	Chrome/Mo Alloy	Outside Scope	3.9	0.8
Furnace 3	Process furnace	Chrome/Mo Alloy	Outside Scope	0.8	0.2
Flash Drum 1	Flash Drum	SS	90	~	0.2
Flash Drum 2	Flash Drum	SS	9.7	~	0.6

3.2 Fixed-Capital Summary

For our economic analysis, our most important cost is the fixed capital of the project as it gives us a strong estimate for the front end payments that the constructed plant will have. The inside battery limit (ISBL) costs, contained within this section, consider the total cost of procurement and installation of equipment for plant designs with a PSA system. The ISBL calculations include furnaces and coolers used to heat and cool inlet streams to reactor and separation conditions, 1 pyrolysis furnace used to ensure isothermal reactor operation, pressure vessels used as the PFR or flash drums, and a separation system containing two distillation columns and two PSA systems.

The total ISBL cost for the design including the PSA was $45 MM. This value consists of a heat exchanger network and separation system containing: 2 PSA systems valued at $3.3 MM, a PFR valued at $0.3 MM (not shown, < 1% ISBL), distillation columns valued at $4.1 MM, 2 flash drums valued at $0.9 MM, 2 process furnaces and a pyrolysis furnace valued at $6.7 MM. These ISBL fractions are illustrated in a pie chart in Figure 5. A preliminary value for the outside battery limit (OSBL) was estimated at 40% of the ISBL[5]. A comprehensive ISBL and OSBL calculation and description is shown in Appendix F.
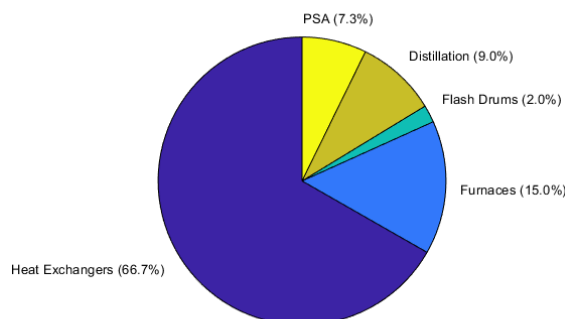

Figure 5. A pie chart showing the fractions of different equipment relative to the total ISBL of $45MM for a process including a PSA system.

Total fixed capital cost (TFCC) was approximately 228% of the ISBL[1]. The TFCC is estimated to be $103 MM for a plant including a PSA. The TFCC includes ISBL, OSBL (40% of ISBL), a contingency (25% of ISBL+OSBL), and indirect costs (30% of contingency+ISBL+OSBL). The total capital investment for this plant is $112.4 MM. These assumptions are used to provide an early estimate based on preliminary equipment costing due to their simplicity. Economic modeling requires more detailed cost correlation which is outside the scope of this report. This economic model is described in detail in Appendix F.

3.3 Discounted Cash Flow Analysis

The discounted cash flow of our proposed process design was compiled after concluding equipment costing and determining variable costs of production. We assumed a 10 year linear depreciation model when accounting for equipment depreciation. A salvage value of 5% of the TFCC was added to the last year of the plant revenue which represents selling the plant. This

discounted cash flow can be translated to an NPV over each year of the project and gives a general estimate for the value gained depending on the lifetime of the chemical plant. Figure 5 shows that with our completed level 5 design we accrue a NPV of \$124.4 MM after year 18.
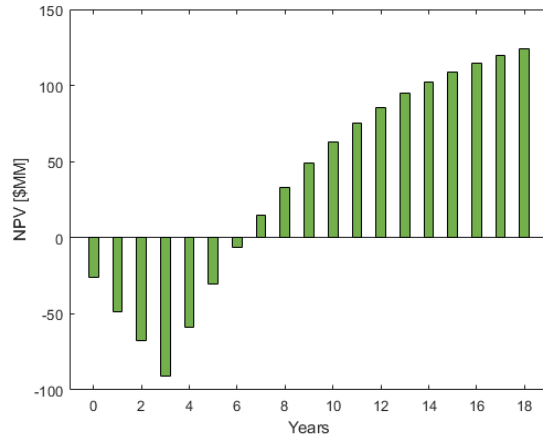

Figure 6: Bar graph showing the discounted cash flow of our project as an NPV across the 15 year plant production life including the 3 years of construction startup.

3.4 Profitability Metrics and Analysis

The profitability of this preliminary design arises from metrics such as production rate and associated prices; however, it is especially weighted on the energy consumption, the natural gas cost, and CO_2 sequestration tax. The typical operating expenses include CO_2 sequestration tax, natural gas cost, refrigerant costs, electricity, fresh ethane and steam cost, and administrative costs (5% of the overall revenue). A pie chart demonstrating the relative percentages of operating costs is shown in Figure 7.
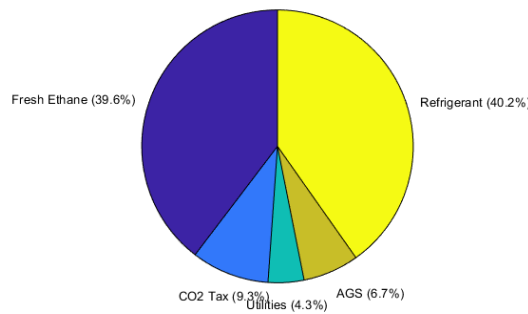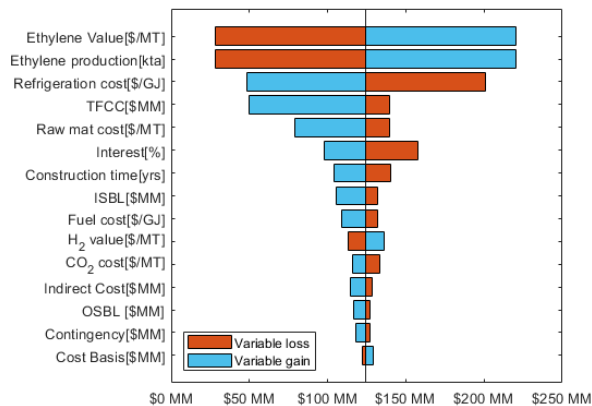

Figure 7. Typical operating costs of our designed plant with a PSA system

| | 8A. | | 8B. |

Figure 8. 8A. NPV sensitivity analysis for our preliminary design with baseline NPV equivalent to 124.4$MM. **8B.** Variable adjustment table showing the defined range of variation in our given variables for the analysis.

We performed a sensitivity analysis and formulated the baseline economic flowsheets (Appendix F.7 and F.8) using excel to have a complete reference sheet to calculate the effects of changes in specific economic variables on NPV. In Figure 8A the NPV of the plant is shown in a tornado plot with varying values of what we deemed were the most important parameters at this later level of design. Additionally, Figure 8B shows the ranges of variation for each parameter used in the tornado plot. The value and production rate of ethylene have the greatest impact on the NPV of the plant, however the next most important variable is the cost of refrigeration across the plant. It is important to note that the NPV becomes zero if refrigeration costs increase by 81%. The TFCC has the potential to decrease NPV by around 60% if it were to double. The ISBL and OSBL are varied independently of other capital costs and have little impact on the overall NPV allowing for flexibility in pricing of the equipment. Specifically for the water PSA cost estimation, we chose a cost of energy to be $0.75/W and a minimum thermodynamic work efficiency scaling factor of 35 which provides a median cost of this separation system. Our sensitivity analysis shows that variations in our selected plant variables provide profitability across a wide range of values. However, this list is not exhaustive and also does not take into account potential compounded changes, such as drop in ethylene price and increased construction time occurring at the same time or a recession.

Our economic model predicts the minimum price of ethylene which produces a profitable plant to be $667/MT. When compared to the current expected price and potential variations, we see this value to be ~30% lower than the assumed sale price and outside the tested range implemented in the sensitivity analysis[7]. This shows that this design is well within sensitivity limits for product value to maintain profitability.

4 HAZOP and Environmental Impact

In our chemical plant development, a Hazard and Operability Study (HAZOP) was conducted while focused on safety and efficiency. Key areas of consideration included the

furnaces, pyrolysis reactor, plug flow reactor (PFR), distillation columns, flash drums, pumps, and pressure swing adsorption (PSA) systems. For the pyrolysis furnace, risks from temperature deviations are identified as most significant. Recommendations include advanced temperature control, alarms, automatic shutdown, maintenance, and operator training. The PFR risks involve temperature and pressure deviations. Mitigation of this includes advanced control systems, safety valves, rupture discs, and scheduled maintenance/monitoring. The flash drums's risks include leakage and blockage. Mitigation involves high-integrity seals, pressure testing, cleaning protocols, pressure relief, and bypass systems. For the PSA system, risks of adsorbent failure and valve malfunction were noted as significant. Mitigation includes monitoring, maintenance, high-quality valves, and operator training. Cooler unit risks included fluid solidification and product/equipment degradation. Mitigation involves temperature alarms, automated controls, calibration, and backup cooling units. Heat exchanger risks included overheating, fouling, and vaporization within shell and tube heat exchangers. Mitigation involves alarms, automatic shut offs, testing, maintenance, low-temperature alarms, auxiliary heaters, and pressure relief. Distillation tower risks included temperature fluctuations, pressure extremes, and flow inconsistencies. Mitigation involves alarms, cooling systems, safety training, vacuum breakers, flow control, and regular checks. Pump risks included flow, pressure, and temperature concerns. Mitigation involves inspections, flow meters, backup pumps, maintenance, and temperature monitoring. An extensive HAZOP is shown in Appendix H and Environmental impact is shown in Appendix G.

5 Process Alternatives and Next Steps

The main assumptions made up to level 5 in the Douglas hierarchy of design is that our plant has no heat loss to the surroundings, the PFR is ideal, and only the provided kinetics are active at these conditions. Additionally, the heat duty required for any operation is ideal and only requires the minimum amount of fuel to operate, the separation system has no heat losses, and operates according to HYSYS. Now that we have moved forward with the analysis, we see that these assumptions need to be verified via experiment prior to plant start up. Pressure drop through the plant, piping/tubing specifications along with heat loss to surroundings, and safety valves/controllers need to be considered in the next steps of this plant design.

Another potential process alternative includes using a third flash drum after the first hydrogen flash equipped with an adiabatic expansion nozzle which can reduce the temperature of the effluent stream to about -210 C and separate hydrogen to the required wt % purity.

We recommended conducting experiments on the reaction chemistry at temperatures above 825°C. This may lead to enhanced ethylene selectivity as there is a trend of increasing selectivity with increasing temperature as shown from our MATLAB conceptual design. A greater range of understanding for the reaction kinetics is required as there are large temperature variations from the studied ranges within plant startup and shutdown[4]. As well, experiments about minimizing the molar ratio of steam to ethane in the reactor should be conducted to

maximize the useful volume of the reactor without allowing for coking buildup as we see NPV increase with lowering the steam-to-ethane molar ratio. Pressure drop experiments should also be conducted to determine real pressure drop through the reactor and its effect on conversion and reaction studies as well as pressure drop through other unit operations across the plant.

6 Conclusion

The techno-economic analysis conducted for a steam ethane cracker designed to produce 200 kta of polymer-grade ethylene is estimated to have an NPV of $124.4 MM. The proposed design leverages optimal reactor conditions including: a volume of 16 m^3, an operating temperature of 825°C, pressure of 2 bar, and an inlet steam-to-ethane molar ratio of 0.6, to achieve a single pass ethane conversion rate of 73%. The PSA system enhances the plant's profitability by allowing the sale of hydrogen as a coproduct. Economic analyses predict a total capital investment (TCI) of $112 million and an internal rate of return (IRR) of 32%.

This economic potential is supported by a detailed market analysis, demonstrating a growing demand for ethylene and hydrogen, alongside an in-depth reaction chemistry review and process simulation in MATLAB and Aspen Hysys. Energy requirements and environmental considerations are addressed with an estimated energy requirement of 14 MJ per kg of ethylene product, and a focus on CO_2 sequestration aligns the project with BICC's sustainability goals. The analysis acknowledges the limitations inherent in preliminary design and suggests further steps for optimization and detailed design, including exploration of reaction chemistry under varied conditions.

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Appendix

A - Additional Figures
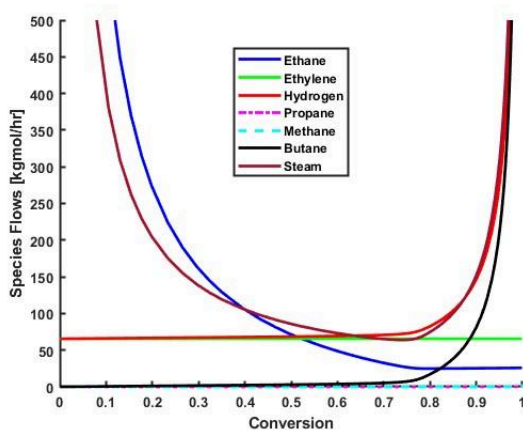
Figure A1. Product Flows vs. Conversion
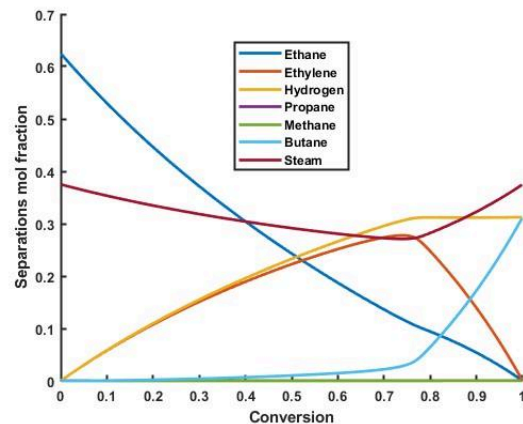
Figure A2. Mol Fraction to separation system
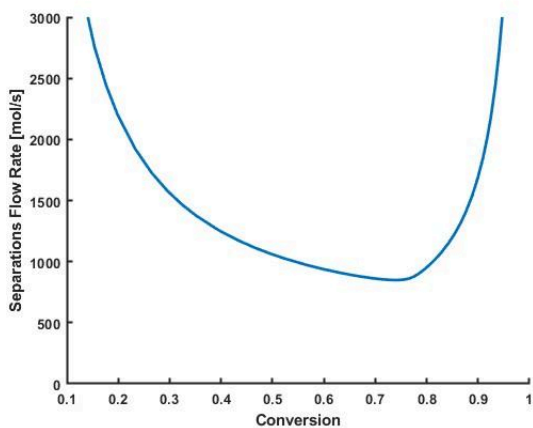
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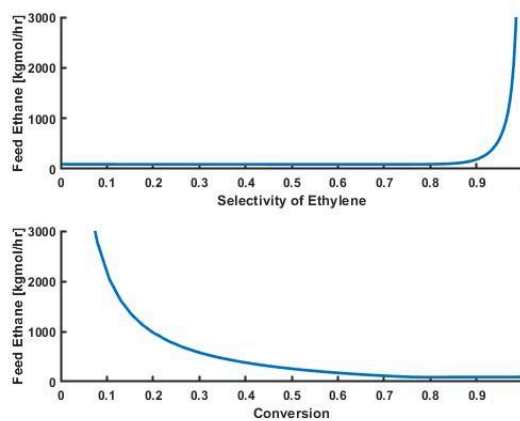
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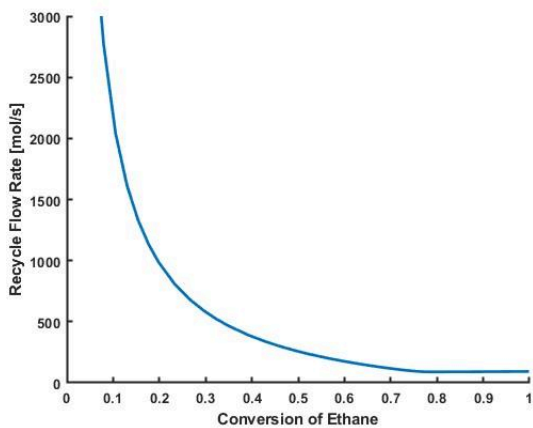
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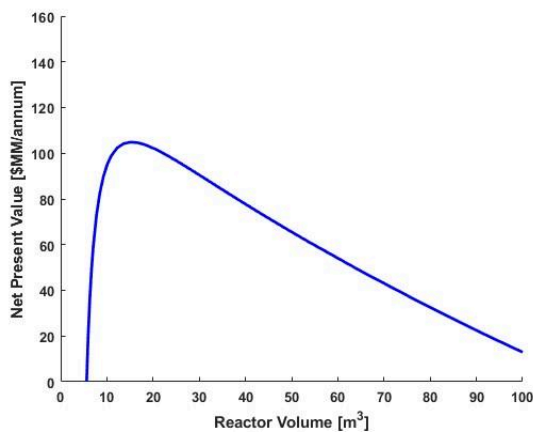
Figure A6. NPV vs. reactor volume [L] for a PFR with no PSA with an operating pressure of 2 bar and temperature of 825 C and steam-to-ethane molar ratio of 0.6.
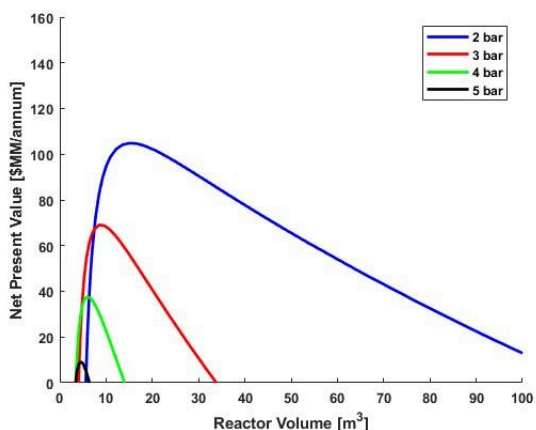
Figure A7. NPV vs. reactor volume [L] for a PFR with no PSA with a varying operating pressure of 2 -5 bar and at a temperature of 825 C and steam-to-ethane molar ratio of 0.6.
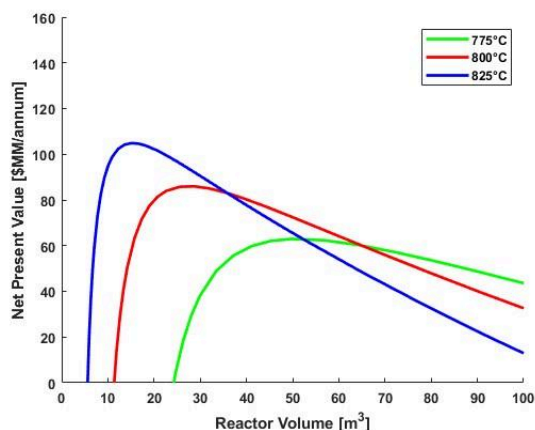
Figure A8. NPV vs. reactor volume [L] for a PFR with no PSA with a varying operating temperature of 775-825C at an operating pressure of 2 bar and steam-to-ethane molar ratio of 0.6.
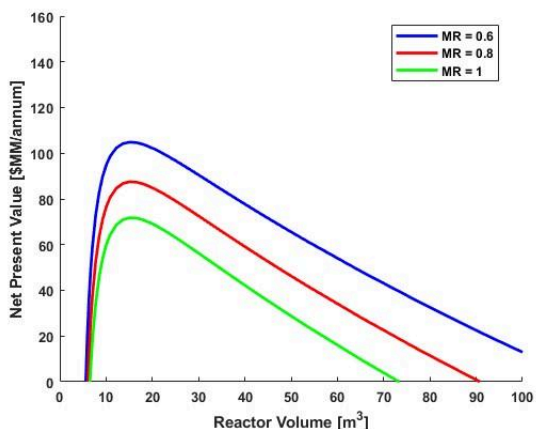
Figure A9. Reactor volume [L] vs. conversion of ethane with no PSA. A finite volume is required at 0 conversion due to the specified production rate of ethylene (200kta)
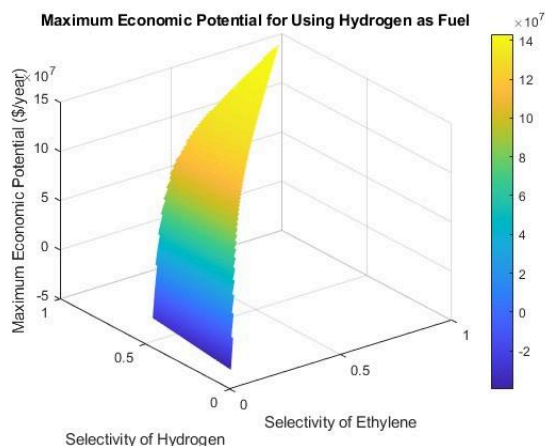
Figure A10: Maximum EP for using hydrogen as fuel: $146 MM, at Selectivity of Ethylene of 1 and Selectivity of Hydrogen of 1.
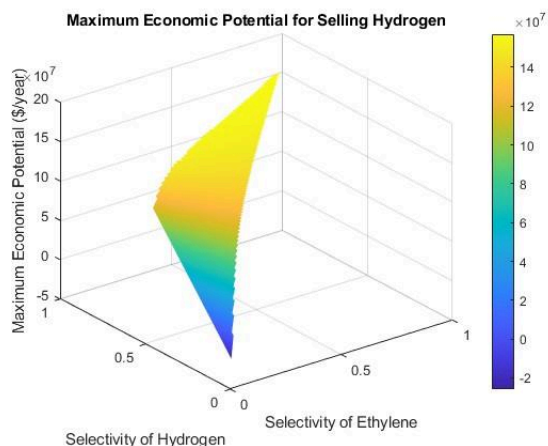
Figure A11: Maximum EP for selling hydrogen as a chemical: $157 MM, at Selectivity of Ethylene of 1 and Selectivity of Hydrogen of 1.

B - Relevant Physical Properties

Property	Ethane (C_2H_6)	Ethylene (C_2H_4)	Hydrogen (H_2)	Propane (C_3H_8)	Methane (CH_4)	Butane (C_4H_{10})
Molecular Formula	C_2H_6	C_2H_4	H_2	C_3H_8	CH_4	C_4H_{10}
Molecular Weight (g/mol)	30.07	28.05	2.016	44.09	16.04	58.12
Boiling Point (°C)	-88.6	-103.7	-252.9	-42.1	-161.5	-0.5
Melting Point (°C)	-183.3	-169.2	-259.2	-187.7	-182.5	-138.4
Density (kg/m³ at STP)	1.356	1.178	0.08988	2.009	0.717	2.48
Critical Temperature (°C)	32.17	9.21	-239.9	96.7	-82.3	152
Critical Pressure (MPa)	4.88	5.04	1.29	4.25	4.60	3.80
Vapor Pressure at 25°C (kPa)	3,844	5,632	20,390	854	4,600	230

Specific Gravity (relative to air)	1.0487	0.968	0.0695	1.56	0.554	2.07
Solubility in Water (mg/L at STP)	61.1	Slightly soluble	Slightly soluble	Slightly soluble	Slightly soluble	Slightly soluble
Odor	Odorless	Sweet, ether-like	Odorless	Odorless	Odorless	Odorless
Flammability	Highly flammable	Highly flammable	Highly flammable	Highly flammable	Highly flammable	Highly flammable
Explosive Limits in Air (vol %)	3.0-12.5	2.7-36	4.0-74.2	2.1-9.5	5.0-15.0	1.8-8.4
Autoignition Temp. (°C)	472	425	571	470	537	405
Toxicity	Simple asphyxiant	Simple asphyxiant	Simple asphyxiant	Simple asphyxiant	Simple asphyxiant	Simple asphyxiant
CAS Number	74-84-0	74-85-1	1333-74-0	74-98-6	74-82-8	106-97-8
Viscosity (μPa·s at 0°C)	8.02	8.52	8.76	7.38	10.96	7.38
Heat of Combustion (MJ/kg)	51.9	49.07	141.88	50.35	55.5	49.5

C - Thermodynamics and Reaction Models

C.1 - Reaction Kinetics

$$C_2H_6 \rightleftharpoons C_2H_4 + H_2 \qquad (1)$$

$$2C_2H_6 \rightarrow C_3H_8 + CH_4 \qquad (2)$$

$$C_2H_6 + C_2H_4 \rightarrow C_4H_{10} \qquad (3)$$

$$r_1 = k_{1,f}[C_2H_6] - k_{1,r}[C_2H_4][H_2] \qquad (4)$$

$$r_2 = k_2[C_2H_6]^2 \qquad (5)$$

$$r_3 = k_3[C_2H_6][C_2H_4] \qquad (6)$$

$$k_{1,f} = 4.652 \times 10^{13} \exp(-273,000/RT) \qquad (7)$$

$$k_{1,r} = 9.91 \times 10^8 \exp(-137,800/RT) \qquad (8)$$

$$k_2 = 3.85 \times 10^{11} \exp(-273,000/RT) \qquad (9)$$

$$k_3 = 7.083 \times 10^{13} \exp(-252,600/RT) \qquad (10)$$

In creating a CO2-neutral process for producing ethylene through thermal steam cracking of ethane, we used kinetic reactions to enhance ethylene yields. The method relied on kinetic models to convert ethane into ethylene and subsequently into heavier hydrocarbons, with Arrhenius rate equations on the reactions' behavior.

We analyzed rate constants k_1, k_{-1}, k_2, and k_3 for primary and secondary reactions, aiding in reactor performance simulation across various conditions of temperature, pressure, molar ratio of steam to ethane, and reactor volume. These constants, based on data from BICC, Inc., allowed for accurate predictions of the steam cracking process's outcomes through the PFR simulations.

By integrating these kinetic formulas into our reactor design, we could simulate interactions between reactants and assess how ethylene production responded to adjustments in temperature, as well as reactant and product levels. This step was vital for transitioning the process from laboratory to pilot scale, providing essential data for BICC's financial assessments regarding the new ethylene production facility.

C.2 - Underwood Equation for Distillation Parameters

To begin distillation design we first determine the feed composition and flow rate as well as assign a q (saturated liquid/vapor parameter). Then from our components that are to enter the column we decide how we want them to be split ie: A/BC if we wanted A to be isolated from B and C. With this split, we then assume full separation of light key into distillate and full separation of heavy key into the bottoms. This also means lighter than light and heavier than heavy keys follow as well. We then determine an r_{min}(minimum reflux ratio) from given equations using relative volatilities (*a*) of each component referenced to the light key as if it were binary distillation[20]. This minimum reflux ratio is then given a factor to account for real separation and gives a reflux ratio of ~1.5-2 times more. A reboiler ratio (*s*) is then found according to the equation below.

$$s = \frac{D}{B}(r + q) - (1 - q)$$

Equation C.2.1

Here, D is the distillate molar flow rate, B is the bottoms molar flow rate, r is the real reflux ratio, and q is the previously mentioned enthalpy parameter. From here, using the FUG method, we can derive an N_{min} by comparing the Eduljee equation to the Gilliland correlation. This Eduljee equation is as follows.

$$\frac{N - N_{min}}{N+1} = 0.75\left[1 - \left(\frac{r - r_{min}}{r+1}\right)^{0.5688}\right]$$

Equation C.2.2

After getting an N_{min}, an N_{real} is determined by $N_{real} = 2N_{min}$. These column parameters were then used as our baseline values for design of distillation columns.

D - Level 1-5 Decisions and Mole Balances

Level 1 Decisions

At Level 1, the primary objective is to establish the fundamental conceptual design of the process. This includes critical evaluations regarding the process's overall viability and the selection of a method for implementation. Our choice to employ thermal steam cracking of ethane for ethylene production is a pivotal Level 1 decision. This selection is based on a comprehensive review of historical data, economic viability, and the ready availability of ethane as a feedstock.

Level 2 Decisions

Level 2 decisions are centered on detailing the chemical processes and the stoichiometric balances of the key reactions transforming ethane into ethylene. This stage involves selecting the basic reaction mechanisms, identifying the optimal conditions for achieving targeted yields, and ensuring the ethylene produced meets required purity standards. Our analysis at this level incorporates kinetic data and thermodynamic principles to understand how these reactions operate efficiently under specific conditions.

Level 3 Decisions

At Level 3, the focus shifts to the process's optimization through the integration of recycle streams, aiming to enhance efficiency and maximize the use of resources. A significant assumption made at this stage is the complete recycling of ethane back into the reactor, which informs our strategy for managing byproducts and unused feedstocks. Design efforts at this level aim to increase ethylene yield and minimize waste. Additionally, evaluating and refining the application of pressure swing adsorption (PSA) technology for separating hydrogen and methane plays a crucial role in our decision-making process at Level 3.

Level 4 Decisions

At level 4, our conceptual design begins the inclusion of energy balances across the plant for the in depth separation system. This considers both outsourced energy for reactor and

separation demands.. The main assumption with this is that no heat is being lost to the surroundings wherever there is an introduction of energy or heat transfer. The objective of this level of design is to specify the direction of separation equipment and optimize on sizing and capex/opex for the separation equipment

Level 5 Decisions

For level 5, our design aims to consider an overall energy balanced over the plant for streams. This becomes a question of heat exchanger integration and optimal heat transfer across the plant. We assume that heat losses from equipment and fouling is negligible at this point and focus on the ideal cases of heat exchangers and stream energy duty.

Mole Balance

Given Reactions

$$C_2H_6 \rightleftharpoons C_2H_4 + H_2 \tag{1}$$
$$\text{Eth} \rightleftharpoons \text{Ethyl} + \text{H}$$
$$2C_2H_6 \rightarrow C_3H_8 + CH_4 \tag{2}$$
$$2\text{Eth} \rightarrow \text{P} + \text{M}$$
$$C_2H_6 + C_2H_4 \rightarrow C_4H_{10} \tag{3}$$
$$\text{Eth} + \text{Ethyl} \rightarrow \text{B}$$
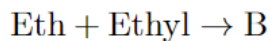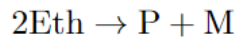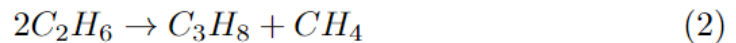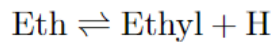
Equation D.1

Initial Mole Balance Matrix:

			Rxn 1, For	Rxn 1, Rev	Rxn 2	Rxn 3
F_{Ethyl}		P_{Ethyl}	1	-1	0	-1
F_P		P_P	0	0	1	0
F_B	-	P_B	+ 0	0	0	1
F_{Eth}		P_{Eth}	-1	1	-2	-1
F_M		P_M	0	0	1	0
F_H		P_H	1	1	0	0

Table D.2

Initial Mole Balance:

$$Ethylene: F_{Ethyl} - P_{Ethyl} + \xi_1 - \xi_3 = 0$$

$$Propane: F_P - P_P + \xi_2 = 0$$

$$Butane: F_B - P_B + \xi_3 = 0$$

$$Ethane: F_{Eth} - P_{Eth} - \xi_1 - 2\xi_2 - \xi_3 = 0$$

$$Methane: F_M - P_M + \xi_2 = 0$$

$$Hydrogen: F_B - P_B + \xi_1 = 0$$

Flows set to zero where appropriate:

				Rxn 1, For	Rxn 1, Rev	Rxn 2	Rxn 3
0		P_{Ethyl}		1	-1	0	-1
0		P_P		0	0	1	0
0	-	P_B	+	0	0	0	1
F_{Eth}		0		-1	1	-2	-1
0		P_M		0	0	1	0
0		P_H		1	1	0	0

Following Balance:

$$Ethylene: - P_{Ethyl} + \xi_1 - \xi_3 = 0$$

$$Propane: - P_P + \xi_2 = 0$$

$$Butane: - P_B + \xi_3 = 0$$

$$Ethane: F_{Eth} - \xi_1 - 2\xi_2 - \xi_3 = 0$$

$$Methane: - P_M + \xi_2 = 0$$

$$Hydrogen: - P_H + \xi_1 = 0$$

Specifications:

$$Ethylene: P_{Ethyl} = 200 \, kta$$

$$Selectivity: S_1 = \frac{P_{Ethyl}}{F_{Eth}}, \, S_2 = \frac{P_{Ethyl}}{F_{Eth}}$$

Final Molar Flows:

$$Ethylene: P_{Ethyl} = 200 \, kta$$

$$\text{Propane: } P_P = \frac{F_{Eth}}{2}(1 - 2S_2 + S_1)$$

$$\text{Butane: } P_B = F_{Eth}(S_2 - S_1)$$

$$\text{Ethane: } F_{Eth} = \frac{P_{Ethyl}}{S_1}$$

$$\text{Methane: } P_M = P_P$$

$$\text{Hydrogen: } P_H = F_{Eth}S_2$$

E - Equipment Design Summary and Hysys Process Flow Diagram

E.1 - Plug Flow Reactor (PFR) Design

The performance of a PFR is based on the assumption that the flow through the reactor does not mix and has a uniform velocity profile. The design equations for the PFR are derived from the molar flow rate balances and the reaction kinetics. The rate of conversion for the PFR is determined using the following design equation:

$$-\frac{dF_A}{dV} = r_A$$

Equation E.1.1

where F_A is the molar flow rate of species A, V is the volume of the reactor, and r_A is the rate of reaction per unit volume for species A. For isothermal reactor conditions, the temperature dependency of the rate can be omitted.

The length of the PFR, which correlates to the residence time required for the desired conversion, is given by integrating the design equation over the reactor volume:

$$L = \int_{F_{AO}}^{F_A} \frac{dF_A}{-r_A}$$

Equation E.1.2

The installed cost of the PFR can be estimated from the reactor volume and material of construction:

$$Installed\ Cost\ (\$) = \left(\frac{M\&S}{280}\right) * 101.9 * D^{1.066} * H^{0.82} * \left(2.18 + F_c\right)$$

$$\text{Where, } F_c = F_m F_p$$

Equation E.1.3

Where M&S is the Marshall and Swift equivalent to 1800 for the year of 2024, D is the diameter of the PFR, H is the length of the PFR, F_m is the material correction factor (2.25 for our case of a stainless steel clad PFR), and F_p is the pressure correction factor (which is 1 due to operating pressure being below 50 psig)

E.2 - Separator / Splitter Design

The separation system design is intended for reactor effluent to be divided into recycle streams, product streams, and fuel streams. For the scope of this preliminary design, the entire separation system is considered as one black box that has outlet streams that split our desired products perfectly. For our system we have six outlet streams from our separators that give a stream for steam, propane and butane, hydrogen, methane, ethane, and ethylene. The perfect splitting gives each of these streams a mol fraction of 1 aside from the mixed stream of propane and butane where each respective mol fraction is based on the reaction rates discussed earlier.

The streams of our separation system, which includes PSA, is defined as follows: F_1 is ethane, F_2 is ethylene, F_3 is the propane and butane mix, F_4 is hydrogen off the PSA, F_5 is the methane off the PSA, and F_6 is the steam separated from the effluent.

The following equation is how we analyzed the costing of our black box separation system including PSA:

$$W_{min} = \sum_i F_i RT_i (\sum_j x_j^i ln\left(\frac{x_j^i}{z_j}\right))$$
$$OPEX(\$/annum) = \lambda \bullet \epsilon W_{min}$$

Equation E.2.1

$$CAPEX(\$) = C_{en}\left(\lambda \bullet W_{min}\right)$$

Equation E.2.2

Where, the summation over i is each different flow and the summation over j is each different species. (the species are assigned numbers in this order: Ethane, Ethylene, Hydrogen, Propane, Methane, Butane, Steam). Additionally, λ is a correction factor which considers normal efficiencies for separation systems, and ϵ is the cost of energy in $/GJ. These values are 35 and 3$/GJ respectively for our case.

The capital expense of the separation system is given in Equation E.2.2 where C_{en} is the cost of energy in $/W and is equivalent to 1$/W.

E.3 - Reactor furnace design

For our reactor furnace, we designed it based on the necessary heat duty required to maintain isothermal conditions inside the PFR assuming complete transfer of heat from the furnace to the reactor contents. This ideal heat transfer assumption is effective at this stage of design and follows the equation below:

$$Installed\ Cost\ (\$) = \left(\frac{M\&S}{280}\right)\left(5.52 \times 10^3\right)Q^{0.85}\left(1.27 + F_c\right)$$
$$Where,\ F_c = F_d + F_m + F_p$$

Equation E.3.1

Here, Q is the absorbed heat duty in units of 10^6 BTU/hr, F_d is the design factor (equivalent to 1.1 in our case since it is a pyrolysis furnace), F_m is the material factor (0.75 in our case for a stainless steel furnace), and F_p being the pressure factor (equivalent to 0 in this case to since our process operates below 500 psi).

E.4 - Heat exchanger design

For each of the heat exchangers across the plant, including the reboilers and condensers of the distillation columns that will be discussed after this, were designed along what required Ua would be needed to promote heat transfer at a maximum temperature along the equipment of 120°C. This cost correlation for the heat exchangers is as follows:

$$Installed\ Cost\ (\$)\ = \left(\frac{M\&S}{280}\right)\left(101.3 * A^{0.65} * F_c\right)$$
$$Where,\ F_c = \left(F_d + F_p\right)F_m$$

Equation E.4.1

Here A corresponds to the contact area between the hot and cold fluid of the respective heat exchanger. For our 6 heat exchangers, they have a contact area of: 25,000ft^2, 25,000ft^2, 25,000ft^2, 6,500ft^2, and 3150ft^2. F_d is the style of heat exchanger cost parameter, F_p is the pressure rating parameter, and F_m is the material choice parameter. All heat exchangers used were U-tube with stainless steel shells and tubes but had varying pressure ratings from 1-80 bar. Thus giving cost parameters of: 0.85, 3.75, and 0-0.55 for F_d, F_m, and F_p respectively.

E.5 - Distillation tower design

Our design on distillation towers was based on the Underwood equation considering the relative volatilities of the main components that are expected in each tower. From this we determined an "ideal" reflux ratio, boil up ratio, and a minimum stages for each distillation tower. From these we systematically varied the calculated values to derive a more optimized cost for the equipment and have a lower energy cost. The costing of distillation towers is a combination of the pressure vessel costing, for the tower shell, heat exchanger costings, for the reboiler and condenser, and tray costing, for the trays inside. The installation cost for these towers is as follows:

Pressure vessel costing:
The costing of the pressure vessel is exactly the same as the equation used for the PFR pressure vessel, however the F_p parameter changes to account for the operating pressure of each column.

Heat exchanger costing:

The costing of the heat exchangers were done by using equation D.4.1 and the same costing parameters with the only change being in the operating pressure where we rated them to operate up to 16 bar.

      Tray costing:

Trays were costed under the assumption that we were using sieve trays with 24 inch spacing and tray material of stainless steel. The installed cost is shown below.

$$Installed\ Cost\ (\$)\ =\ \left(\frac{M\&S}{280}\right)\left(4.7\ *\ D^{1.55}\ *\ H\ *\ F_c\right)$$

$$Where,\ F_c\ =\ F_s + F_t + F_m$$

Equation E.5.1

In this equation, D is the diameter of the trays in feet, H is the height of the stacked trays of the total column, and each of the F parameters correspond to the spacing, tray type, and material of the trays, each of which are 1 for 24in tray spacing, 0 for sieve trays, and 1.7 for stainless steel respectively.

E.6 - Hydrogen PSA Design

      The hydrogen PSA system was designed based on the following methane adsorption isotherm and assumes that all of the methane adsorbs to the zeolite with 95% loading within 300s after pressurization. We assume that other materials (ethylene, ethane, etc.) adsorb more strongly than methane and therefore basing this PSA off of the methane adsorption is a more conservative design. We pressurize the hydrogen from 2 bar to a maximum of 12.5 bar which produces a change in zeolite loading of 1.05 mol/kg zeolite. We do not pressurize higher than this pressure because hydrogen becomes supercritical at this temperature.
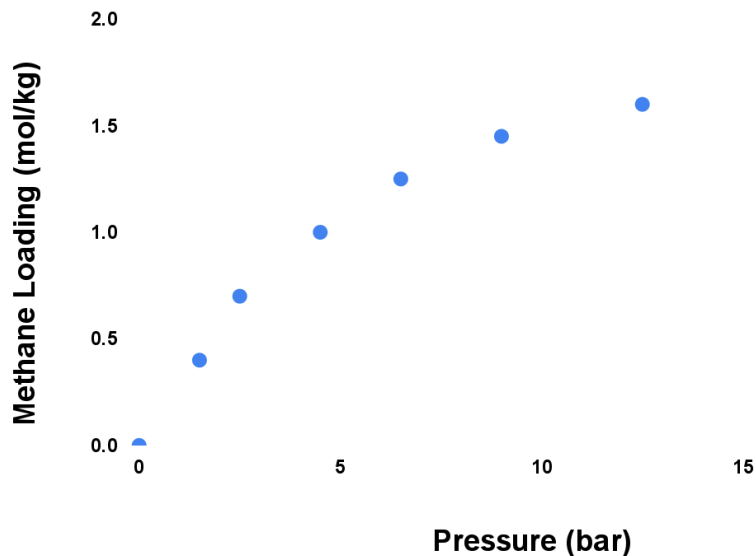
To find the required amount of zeolite per bed we use the following equation:

$$M = \frac{F_{methane}^{out} * t_{adsorption}}{q_{loading} * f_{load}}$$

In which M is the mass of the bed in kg, $F_{methane}{}^{out}$ is the flow of non hydrogen material out of the PSA with trace hydrogen, $t_{adsorption}$ is the time for adsorption, $q_{loading}$ is the amount of material possible to be removed from a pressure swing of 12.5 - 2.5 bar and f_{load} is the load percentage assumes 95 % loading. This zeolite packing is costed as follows:

$$Zeolite\ cost(\$)\ =\ m_{zeolite}\ *\ 5\$/kg\ zeolite$$

We then use 4 PSA drums sized by assuming the bulk density of zeolite is 795 kg/m³ which produces a required volume of 1.24 m³ when we utilize only 80 % of the volume of the drum (to allow for 20 % headspace). The length and diameter of each PSA system is 0.46 m and 0.115 m, respectively. The piping and instrumentation diagram for a model PSA system is shown below:
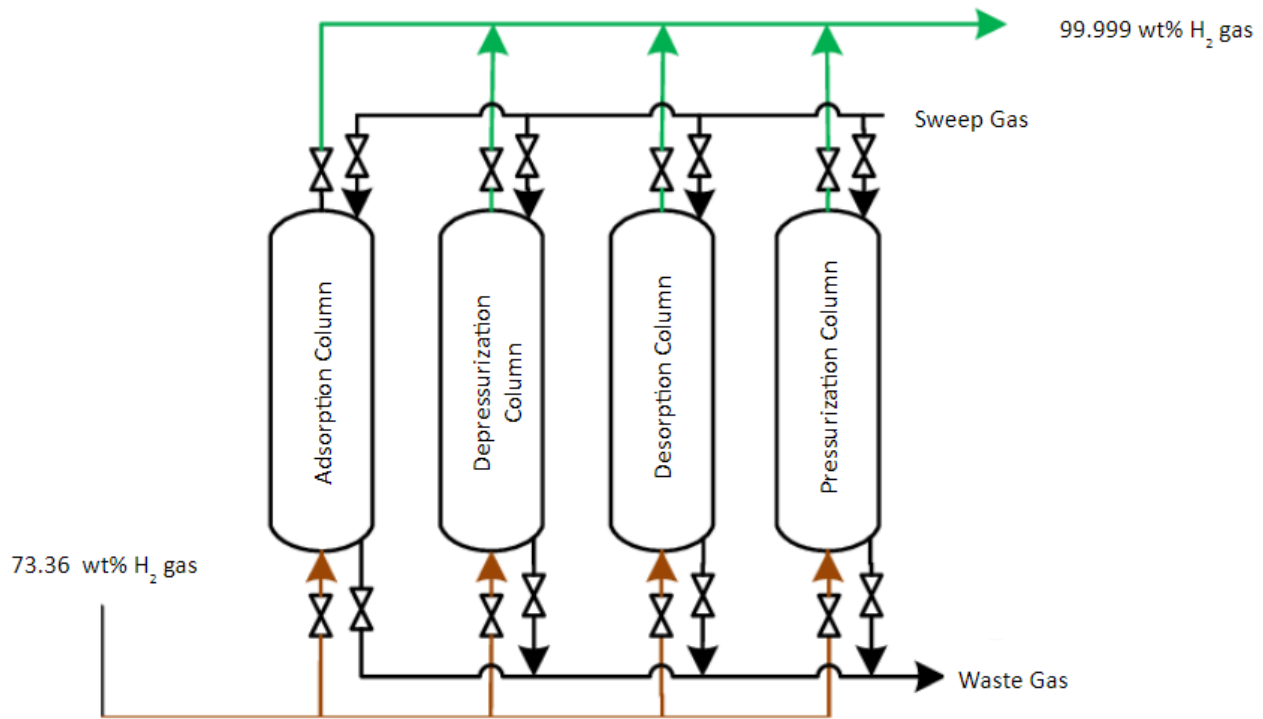
Figure E.6.1: PSA process flow diagram adapted from citation 22, *Biogas Upgrading by Pressure Swing Adsorption*

E.7 - Equipment Table

F - Economic Assumptions, Formulas, and Spreadsheets

For Cap expenses we have an ISBL, OSBL and Contingency which sum up to be our total fixed capital cost (TFCC). For the inside battery limit(ISBL) we made the assumption that

only the installation costs for our equipment would be considered within the scope of this preliminary design since it gives a very strong estimate for the largest costs that are directly integrated into our chemical plant. For the OSBL, we make the assumption that it is equivalent to 40% of the ISBL due to generalized cost estimates from (cite the chem engineering notes where it says this somehow "Econ 1- Motivation and capital costs 2024 dist.pdf"). Contingency, which is our safety and predicted accident money that is set aside, is estimated to be 25% of the sum of ISBL and OSBL. We assume that at year 0, 1 and 2 we spend 25% of the TFCC in each of these years and then spend the last 25% in year 3 along with the entire WC (which is defined as 2 months worth of ethane for full plant production).

The salvage cost of our plant is given as 5% of the TFCC and therefore is taken as a negative cash flow at the end of our plant life (15 years after plant start up) and is added to revenue for the last year in our cash flow.

Our revenue is determined to be the money made from selling ethylene, selling our fuel stream (which is technically used as fuel for our own plant but takes away from fuel price and therefore can be considered a revenue), and selling the Hydrogen stream off PSA as a chemical. As well, our AGS (money towards administration and operators) is given as 5% of our revenue and must then be taken away from profit as a cost of manufacturing. The cost of manufacturing also includes the feedstock price of ethane, teh carbon sequestration price, the natural gas price, and AGS. The difference between revenue and COM is taken as our gross profit.

We determine a taxable income per year by subtracting depreciation of equipment from our gross profit. This depreciation is assumed to be 10 year linear for all equipment bought and the percentage of tax relief is given as:

$$D_i = \frac{cost\ basis}{equipment\ life}$$

$$cost\ basis = \frac{21}{20}(2.28 + ISBL)$$

Equation F.1

From this taxable income, we introduce the tax rate over our plant which is 27% to determine how much we pay in taxes and determine a cash flow using the following equation:

$$Cash\ flow = (REV - COM) * (1 - t) + D$$

Equation F.2

Where, cash flow is a per year, non discounted, after tax value for how much money our process generates. REV is the yearly revenue of our plant, COM is the cost of manufacturing, t is the tax rate, and D is depreciation each year. The present value (PV) is the cash flow at each year divided by the discount factor at each year. The equation is as follows:

$$PV = \frac{Cash\ Flow}{(1 + enterprise\ rate)^n}$$

Equation F.3

Where, enterprise rate is the given value of 15% and n is the year in which each cash flow is from.

This gives a dollar amount of present value of any specific year. This is then used to determine a net present value (NPV) which is calculated as the sum of all previous PVs up to the year that an NPV is calculated at. The equation is as follows:

$$NPV_j = \sum_i^j PV_i$$

Equation F.4

Where, j is the year at which NPV is calculated for, and i is 0 to consider all present values from year 0 onward.

This value of NPV gives a good estimate of whether or not our design will produce positive investment results as dollar values equated to today's dollars even though the profit will come later. This is the most important calculation for the preliminary design and is paramount to deciding whether or not to go forward with the project and eventually benign construction of the chemical plant.
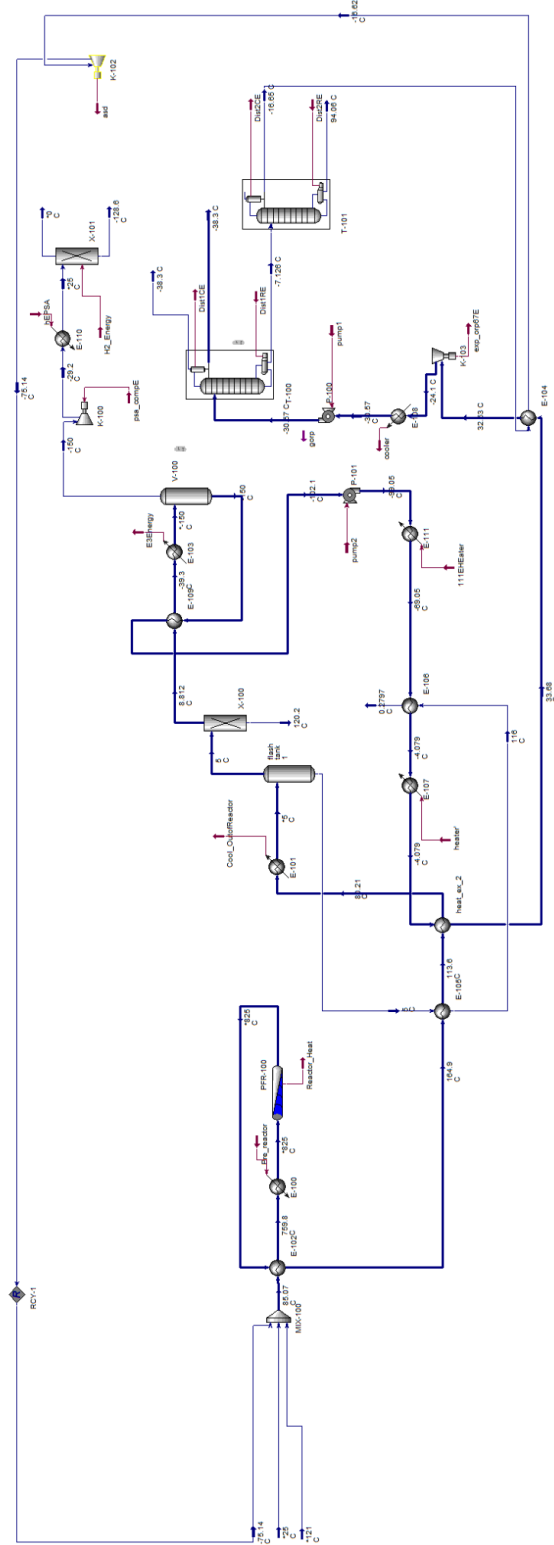
Hysys process flow diagram

Figure F.5

CashFlow Diagram
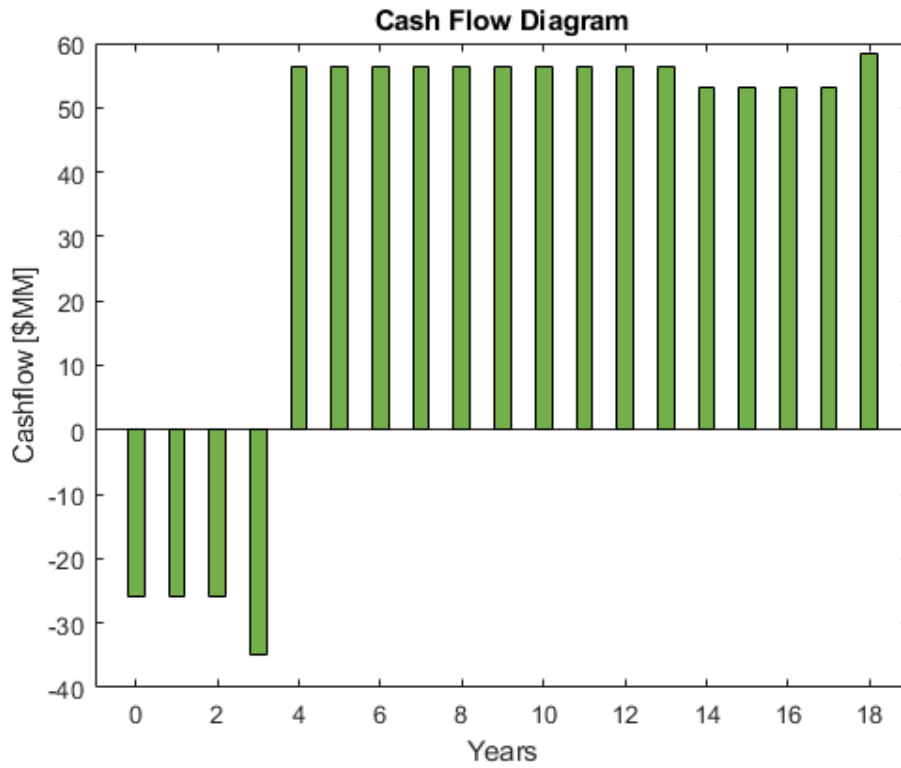
Figure F.6: Cash flow diagram of our preliminary design with PSA separation considered

Economic SpreadSheet

BICC, Inc.
123 Lagoon Road
Santa Barbara, CA

ECONOMIC ANALYSIS

Plant Location
Case Description

Economic Analysis Considering Pressure Swing Adsorption

Rev	Date	BY	APVD	Rev	Date	BY	APVD	
V1.1	4/25/2024	EKT						

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	180.0
Byproduct revenue	28.7
Raw materials cost	53.8
Utilities cost	60.5
Consumables cost	0.0
CO_2 sustainability charge	12.5
VCOP	98.1
Salary and overheads	0.0
Maintenance	0.0
Interest	0.0
AGS	9.0
FCOP	9.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	45.5
OSBL Capital Cost	18.2
Indirect Cost	23.9
Contingency	15.9
Total Fixed Capital Cost	103.4
Working Capital	9.0
Start-up Costs	0.0
Land	0.0
Total Capital Investment	112.4

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% SU	% FCOP	% VCOP
0	25%				
1	25%				
2	25%				
3	25%	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	18 yr	Salvage Value	5%	Cost Basis	114.0262 $MM

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project Year	Cap. Ex.	Revenue	COM	Gr. Profit	Deprcn.	Taxable Inc	Taxes Paid	Cash Flow	PV of CF	NPV	IRR	NV
0	25.9	0.0	0.0	0.0	0.0	0.0	0.0	-25.9	-25.9	-25.9		-25.9
1	25.9	0.0	0.0	0.0	0.0	0.0	0.0	-25.9	-22.5	-48.3		-51.7
2	25.9	0.0	0.0	0.0	0.0	0.0	0.0	-25.9	-19.6	-67.9		-77.6
3	34.8	0.0	0.0	0.0	0.0	0.0	0.0	-34.8	-22.9	-90.8		-112.4
4	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	32.2	-58.6	-27%	-56.1
5	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	28.0	-30.6	0%	0.2
6	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	24.3	-6.3	13%	56.5
7	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	21.2	14.9	20%	112.8
8	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	18.4	33.3	24%	169.1
9	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	16.0	49.3	26%	225.4
10	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	13.9	63.2	28%	281.7
11	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	12.1	75.3	29%	338.0
12	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	10.5	85.8	30%	394.3
13	0.0	180.0	107.1	72.9	11.4	61.5	16.6	56.3	9.2	95.0	31%	450.6
14	0.0	180.0	107.1	72.9	0.0	72.9	19.7	53.2	7.5	102.5	31%	503.8
15	0.0	180.0	107.1	72.9	0.0	72.9	19.7	53.2	6.5	109.1	31%	557.1
16	0.0	180.0	107.1	72.9	0.0	72.9	19.7	53.2	5.7	114.7	32%	610.3
17	0.0	180.0	107.1	72.9	0.0	72.9	19.7	53.2	4.9	119.7	32%	663.5
18	-5.2	180.0	107.1	72.9	0.0	72.9	19.7	58.4	4.7	124.4	32%	721.9

ECONOMIC ANALYSIS

NPV	18 years	124.4 $MM	Total Project IRR	32%
NPV at yr	18	124.4 $MM		

NOTES

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

Figure F.7: Economic spreadsheet for plant design including PSA separation

G - Considerations of Global, Cultural, Social, Environmental, and Economic Factors Related to This Project

Global Factors:

The surge in global ethylene demand, attributable to its applications in sectors such as packaging, construction, and agriculture, aligns with our project's aim to fulfill these market requirements efficiently. Situated on the Gulf Coast, our initiative benefits from prime access to global markets, enhancing export opportunities in the face of fluctuating international oil and gas prices. This location positions us to leverage the anticipated growth in ethylene demand, thereby securing a well used location with infrastructure with many pipelines and shipping lanes.

Cultural and Social Factors:

Our project is poised to drive economic development and create employment opportunities, fostering a positive impact on community relations. Prioritizing engagement with local communities is crucial, ensuring the project resonates with regional social and cultural values. This encompasses a commitment to honor local traditions, contribute to development efforts, and maintain transparent communication with all stakeholders, thereby building a foundation of trust and mutual benefit.

Environmental Factors:

Committing to CO_2 neutrality via carbon capture and storage underscores our dedication to addressing climate change challenges. The application of pressure-swing adsorption technology for CO_2 capture, alongside the innovative use of captured CO_2 and the efficient exploitation of shale ethane, reflects our commitment to sustainability. These measures exemplify our approach to minimizing environmental impact, emphasizing resource efficiency, and promoting waste reduction.

Economic Factors:

The project stands to gain economically from the advantageous cost of shale ethane, coupled with the region's robust infrastructure and technical expertise. These elements, together with the prospect of competitive ethylene pricing and the strategy to secure fixed-price contracts for feedstock, bolster economic resilience and predictability. However, the project's economic viability remains sensitive to the volatility of energy prices and the influence of tax legislation, highlighting the importance of strategic planning and risk management in ensuring long-term success.

H - HAZOP and Safety Data Sheet

HAZOP

Item	Parameter	Guide	Cause	Consequence	Safeguards	Recommendation
PFR Furnace	Temperature	More	Heater Overperf-ormance	Overheating could lead to thermal degradation of reactants/products, unsafe operating conditions.	Temperature control system, high-temperature alarms.	Regular calibration and maintenance of temperature sensors and control systems. Consider installing an automatic shutdown for overheating.
		Less	Heater Underper-formance	Inadequate heating could result in incomplete reactions, accumulation of unreacted feed, and low conversion rates.	Backup heaters, low-temperature alarms.	Implement redundant heating systems and ensure proper insulation to maintain temperature.
	Pressure	More	Blockage or Reaction Byproduct Buildup	Overpressure could result in leaks, equipment rupture, and potential release of hazardous materials.	Pressure relief valves, regular pressure monitoring.	Conduct pressure relief system tests and inspections routinely, train personnel for quick response to pressure deviations.
		Less	Inlet/Outl-et Valve Malfuncti on	Low pressure can cause poor reactant flow, affecting reaction rates and potentially leading to an unsafe vacuum condition.	Vacuum breakers, pressure alarms.	Schedule regular maintenance for valves, and install a control system to maintain minimum pressure

levels.

Splitter						
	Flow	More	Valve Failure Open	Excessive flow can lead to increased reaction rates, potential for runaway reactions, and overpressure.	Flow meters, automatic control valves.	Implement flow control with automatic shutoff capabilities and conduct regular inspections and testing of valves.
		Less	Valve Failure Closed	Reduced flow can lead to low reactant concentrations, poor conversion rates, and potential for overheating in the furnace due to lack of cooling effect of the flow.	Redundant flow paths, flow alarms.	Use fail-open valves and maintain a parallel flow path to ensure continuous operation.
	Feed Flow	More	Valve Stuck Open	Increased flow to one side can cause high pressure, leading to pipe rupture or equipment failure.	Flow monitoring systems	Install automatic shutdown systems for high flow conditions.
		Less	Valve Stuck Closed	Inadequate flow can cause low pressure, leading to poor separation efficiency and process downtime.	Pressure transmitters and alarms	Implement a fail-open control valve to maintain minimum flow.
	Temperature	More	Heater Control Failure	Overheating can cause fluid expansion and high pressure, risking leaks and material degradation.	Temperature control systems	Regular maintenance and inspection of heating elements.
		Less	Heater Control Failure	Too low temperature may increase viscosity, leading to incomplete separation and increased energy costs.	Temperature sensors with alarms	Use a redundant heating system to maintain optimal temperature.
	Pressure	More	Control Valve Failure	High pressure may exceed equipment design limits, leading to equipment failure or hazardous release.	Pressure relief valves	Conduct regular pressure relief system tests and inspections.

Equipment	Parameter	Deviation	Cause	Consequence	Detection	Mitigation
		Less	Inlet Blockage	Low pressure may cause poor separation and system inefficiencies.	Pressure indicators and alarms	Install a bypass line around the splitter for pressure maintenance.
	Composition	Off-spec	Feed Contamination	Inconsistent product quality, could lead to downstream process impacts.	Online composition analyzers	Implement upstream purification steps and regular feedstock quality checks.
		Off-spec	Incorrect Feed Ratio	Suboptimal separation leading to waste of resources and energy.	Regular calibration of flow meters	Use precision control valves and flow meters for accurate feed ratio.
Heater	Temperature	More	Control Failure	Overheating of the stream, potential for thermal degradation of fluids or materials, risk of fire or explosion.	High-temperature alarms, automatic shutdown systems.	Regularly test and maintain temperature control systems, install redundant temperature sensors.
		Less	Control Failure	Underheating of the stream, leading to inadequate process temperatures, possible solidification or increased viscosity of fluids.	Low-temperature alarms, backup heaters.	Implement procedures for heater switch-over in case of failure, ensure proper thermal insulation.
	Flow Rate	More	Valve Stuck Open	Increased flow through heater, potential overheating or hot spots, energy wastage.	Flow control systems, overheat protection systems.	Install flow regulation valves, conduct routine checks on flow meters and control valves.

	Less	Valve Stuck Closed	Reduced flow through heater, poor heat transfer, process inefficiency.	Flow indicators, low-flow alarms.	Use fail-open valves, maintain a bypass line for alternative flow paths in case of valve failure.
Pressure	More	Over pressure	Potential for leaks, pipe rupture, or heater damage.	Pressure relief valves, burst disks.	Regular inspection of pressure relief devices, pressure monitoring.
	Less	InletOutlet Blockage	Inefficient heating, increased strain on heater components.	Pressure gauges, alarms.	Ensure routine maintenance and cleaning to prevent blockages.
Power Supply	Irregular	Power Surge/Fail	Unstable temperatures can lead to process interruption or equipment damage.	Surge protectors, UPS systems.	Install protective devices against surges, maintain backup power supply for critical heater operations.
	Loss	Power Outage	Complete process halt, risk of solidification or cold spots in the system.	Emergency power systems, alarms.	Regularly test backup power systems, ensure quick restoration of power or shutdown procedures.
Speed	More	Control Failure	Over-mixing can lead to shear damage to product, excessive energy consumption, or equipment wear.	Speed control systems, vibration detection systems.	Implement regular maintenance checks on mixer speed controls, install automated shutdown on vibration detection.

Mixer		Less	Control Failure	Under-mixing can result in an inhomogeneous product, affecting quality and downstream processes.	Speed sensors, torque monitoring.	Schedule periodic calibration of speed controls, ensure redundancy in sensing equipment.
	Temperature	More	Heating System Failure	Increased temperature can cause degradation of heat-sensitive materials, off-spec products.	Temperature control systems, thermocouples.	Regular inspection and testing of mixer heating elements, install temperature alarms.
		Less	Heating System Failure	Low temperature may not be sufficient for the reaction of the mixing process, resulting in poor quality.	Temperature gauges, low-temperature alarms.	Utilize a backup heating system, ensure proper thermal insulation.
	Pressure	More	Overfill or Gas Evolution	High pressure can cause seals to fail or create a hazardous environment, possible equipment damage.	Pressure relief devices, monitoring systems.	Conduct regular checks on pressure relief valves, install fail-safe shutdown systems.
		Less	Leak or Inadequate Sealing	Low pressure can result in ingress of contaminants or atmosphere, potentially compromising product quality.	Pressure sensors, leak detection systems.	Ensure regular inspection of seals and gaskets, maintain an inert atmosphere if required.
	Composition	Off-spec	Incorrect Proportion	Inaccurate mixing ratios can lead to an off-spec product, affecting subsequent processes and product quality.	Automated dosing systems, inline composition analysis.	Implement stringent quality control measures, regular calibration of dosing equipment.
		Contamination	Cross contamina	Introduction of foreign materials can result in product spoilage or	Regular cleaning	Schedule regular mixer cleaning,

		on	tion	reactions creating hazardous by-products.	schedules, contaminant monitoring.	enforce strict contamination control protocols.
PSA	Adsorption Pressure	More	Control Valve Failure	High pressure can lead to bed compaction and desorbent losses, potential safety risks from vessel rupture.	Pressure relief valves, safety interlocks.	Install multiple independent pressure relief systems and frequent testing of control valves.
		Less	Leak or Valve Malfuncti-on	Low pressure can cause poor adsorption efficiency, leading to off-spec product and process inefficiency.	Pressure sensors, automatic leak detection.	Conduct regular system integrity checks and maintain a backup control valve.
	Desorption Pressure	More	Regenerat-ion Control Malfuncti-on	Excessive pressure during desorption can lead to desorbent waste and safety risks.	Pressure control systems, alarms.	Regularly calibrate and test pressure controllers, have emergency shutdown procedures in place.
		Less	Improper Regenerat-ion Sequence	Inadequate desorption pressure can result in incomplete regeneration, reduced capacity for the next cycle.	System sequence checks, process timers.	Verify sequence operation regularly and ensure proper staff training on system operation.
	Time	More	Controller Failure	Extended cycle time can reduce throughput and increase wear on valves and adsorbents.	Cycle timers, flow monitors.	Implement strict maintenance schedules for cycle controllers and related equipment.
		Less	Controller	Reduced cycle time may not	System	Regularly review

		Failure	allow complete adsorption or desorption, leading to diminished separation performance.	checks, performance monitoring.	system performance data to ensure optimal cycle timing.
Temperature	More	Heater Failure	High temperatures can cause thermal degradation of the adsorbent material, safety risks.	Temperature sensors, cooling systems.	Monitor temperatures closely, maintain backup cooling capabilities.
	Less	Heater Failure	Low temperatures may lead to poor adsorbate release or increased energy use for regeneration.	Temperature alarms, redundant heaters.	Inspect and maintain heaters, ensure proper insulation to retain heat.
Composition	Off-spec	Feed Contamin-ation	Incorrect feed composition can lead to poor adsorption selectivity, reduced product purity.	Composition monitors, pre-treatment systems.	Implement upstream purification steps, conduct regular feedstock quality checks.
	Varied	Feed Variability	Variation in feed composition can result in fluctuating performance and product quality.	Inline analyzers, control systems adjustments.	Install advanced control systems to adjust process parameters dynamically.
Temperature	Less	Excessive cooling capacity	Fluid solidification, possible blockages	Temperature alarms, automated controls	Regular calibration and maintenance of temperature control systems
	More	Inadequate cooling	Product degradation, failure to meet process specifications	Backup cooling units,	Evaluate cooling capacity and

Cooler	Flow	More	Valve stuck open	Mechanical stress, premature equipment wear	low-temp alarms	redundancy in system design
					Flow meters, automatic shutoff valves	Implement scheduled maintenance and inspections of flow systems
		Less	Valve stuck closed	Reduced cooling effectiveness, potential for overheating	Redundant flow paths, flow alarms	Design system with parallel cooling paths for reliability
	Pressure	More	Blockage or overfilling	Potential for rupture or leaks	Pressure relief valves, routine monitoring	Regular checks for blockages and pressure regulation adherence
		Less	Wear and tear, valve malfunctio n	Inefficient cooling, reduced system effectiveness	Pressure boosters, alarms	Routine inspections and maintenance of pressure components
	Temperature	More	Control system malfunctio	Overheating leading to thermal expansion and stress	High-temp alarms, automatic	Regular testing and maintenance of temperature

Heat Exchanger	Flow	Less	Insufficient heat transfer	Poor process performance, energy inefficiency	Low-temp alarms, auxiliary heaters	Regular performance evaluations and system audits
			n		shutoff	control systems
	Flow	More	Control valve failure open	Increased pressure and flow, leading to mechanical failure	Flow controllers, safety valves	Frequent calibration and maintenance of flow control valves
		Less	Control valve failure closed	Reduced heat transfer efficiency, potential system overheating	Backup flow paths, alarms	Install redundant flow systems for critical operations
	Pressure	More	System overpressure	Equipment stress, possible leaks or ruptures	Pressure relief systems, burst discs	Routine pressure relief system testing and personnel training
		Less	General wear or malfunction	Low pressure leading to inadequate thermal transfer	Pressure indicators, supplementary systems	Periodic checks and maintenance of pressure support systems
	Temperature	More	Heater malfunctio	Degradation of products, potential for column damage	High-temp alarms,	Monitor and maintain

			n		cooling systems	temperature controls, train operators
Distillation Tower		Less	Insufficient heating	Ineffective separation, higher operating costs	Low-temp alarms, additional heaters	Evaluate heating capabilities and incorporate redundancy
	Pressure	More	Excess pressure build-up	Risk of column failure and hazardous material release	Pressure relief valves, safety interlocks	Regular safety valve checks and emergency response training
		Less	Vacuum due to condenser failure	Poor vapor-liquid equilibrium affecting separation efficiency	Vacuum breakers, alarms	Maintain and inspect vacuum prevention devices regularly
	Flow	More	High internal reflux	Flooding of the column, reduced separation efficiency	Flow meters, control valves	Dynamic control of flow rates based on real-time data
		Less	Low internal reflux	Reduced throughput and potential column drying out	Minimum flow controls, flow indicators	Regular flow system checks to ensure continuous operation
	Temperature	More	Heater control	Overheating can lead to fluid degradation	Temperature sensors,	Regular inspection and testing of

Kettle Reboiler			failure		high-temperature alarms	temperature control systems
	Pressure	Less	Insufficient heating	Incomplete vaporization, affecting tower operation	Low-temperature alarms, backup heaters	Ensure adequate heating capacity and system redundancy
		More	Valve failure or blockage	Overpressure can lead to equipment rupture	Pressure relief valves, monitoring systems	Install multiple pressure relief devices and routine inspections
		Less	General wear and tear	Underpressure can cause poor heat transfer	Pressure sensors, alarms	Regular maintenance and checks of pressure components
	Level	More	Feed excess or control failure	Risk of overflow and safety hazards	Level indicators, overflow alarms	Implement automatic level control and regular checks
		Less	Inadequate feed	Low level can expose heating elements and damage them	Low-level alarms, feed control systems	Monitor feed rates and maintain minimum level requirements
	Temperature	More	Cooling failure	Overheating leading to system failure	Temperature alarms,	Regular inspection and maintenance

					automatic shutoff	of cooling systems
Conden ser	Pressure	Less	Excessive cooling	Condensate may freeze, blocking flow	Low-temperat ure alarms, heaters	Monitor cooling rates, install temperature regulation
		More	Overpress ure from blockage	Potential for leaks or condenser rupture	Pressure relief valves, burst disks	Frequent checks and maintenance of pressure relief systems
		Less	Vacuum condition	Air ingress, affecting condensation efficiency	Vacuum breakers, pressure alarms	Ensure integrity of vacuum seals and routine checks
	Flow	More	Valve stuck open	Increased flow can overload the condenser	Flow meters, automatic control valves	Regular calibration of flow control systems
		Less	Valve failure closed	Reduced cooling efficiency	Redundant flow paths, flow alarms	Install parallel pathways for critical operations
	Flow	More	Impeller wear or misalignm ent	Excessive flow can cause system stress	Flow meters, control valves	Regular inspection and maintenance of impeller and alignment
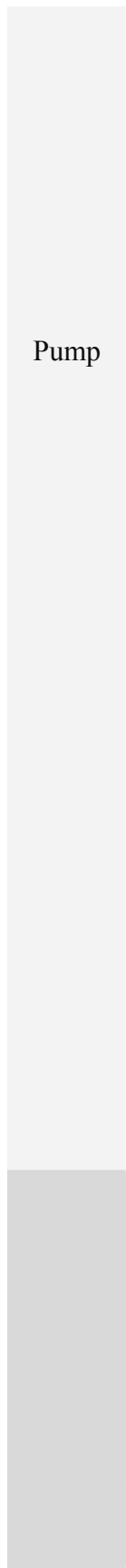
Pump	Pressure	Less	Valve failure or clogging	Reduced flow leading to process inefficiency	Backup pumps, flow alarms	Implement routine cleaning and maintenance schedules
		More	Discharge blockage	Overpressure can damage pump and piping	Pressure relief valves, sensors	Regular checks of discharge lines and relief settings
		Less	Suction pressure drop	Cavitation, leading to mechanical failure	Pressure gauges, low-pressure alarms	Monitor suction conditions and adjust as necessary
	Temperature	More	Overloading or friction	Overheating can lead to seal failure	Temperature sensors, cooling systems	Ensure proper lubrication and cooling of pump system
		Less	Ambient conditions	Low temperatures may cause fluid viscosity increase	Heaters, temperature monitoring	Preheat fluids in cold conditions to maintain viscosity
	Flow	More	Control failure	Excessive speeds can cause mechanical failure	Speed controls, vibration sensors	Regular monitoring and maintenance of speed control systems
		Less	Inlet	Reduced output and efficiency	Inlet filters,	Regular inspection

Expander			blockage		alarms	and cleaning of inlet pathways
	Pressure	More	Upstream pressure increase	Potential for overloading and damage	Pressure relief devices, monitors	Install and maintain upstream pressure regulation
		Less	Leakage or valve failure	Decreased performance, energy loss	Leak detection systems, seals	Routine checks for leaks and integrity of valves
	Temperature	More	Compression heat	Overheating can degrade components	Cooling systems, temperature sensors	Implement cooling measures and monitor temperature closely
		Less	Ambient temperature drop	Material contraction, mechanical issues	Thermal insulation, heaters	Use heaters and insulation to manage temperature effectively

Safety Data Sheet

Species	Flammability	Explosive Limits (v/v)	Toxicology	Corrosiveness
Ethane[17]	Flammable gas	Lower:	Asphyxiant in high concentrations	Non-corrosive

	(Category 1)	3.0%, Upper: 12.4%		
Ethylene[12]	Extremely flammable gas (Category 1)	Lower: 2.7%, Upper: 36.0%	May cause frostbite on contact with liquid form, simple asphyxiant	Non-corrosive
Hydrogen[13]	Extremely flammable gas (Category 1)	Lower: 4.0%, Upper: 75.0%	Non-toxic, simple asphyxiant	Non-corrosive
Methane[14]	Extremely flammable gas (Category 1)	Lower: 5.0%, Upper: 15.0%	Non-toxic, simple asphyxiant in high concentrations	Non-corrosive
Butane[15]	Extremely flammable gas (Category 1)	Lower: 1.8%, Upper: 8.4%	May cause drowsiness or dizziness, simple asphyxiant in high concentrations	Non-corrosive
Propane[16]	Extremely flammable gas (Category 1)	Lower: 2.1%, Upper: 9.5%	Simple asphyxiant in high concentrations	Non-corrosive

I - Code

Getting Flows Function

```
function [vol,flows] = getFETi(F_ETi,Vmax,T,Ptot)
MMs = (3600*24*7*50)/(1e+9) * [30.08, 28.06, 2.02, 44.11, 16.05, 58.14, 18.02];
V0 = 0; %starting volume along reactor length
MR = 0.6; %some molar ratio for steam in units of Mol Et/Mol steam
%constant molar flow rate per year of ethylene
```

```
%Fsteam= F_ETi/MR;
Fsi = [F_ETi; 0; 0; 0; 0; 0; F_ETi*MR]; %inital conditions matrix
Vspan = [V0, Vmax]; %volume in liters,
[V, F] = ode15s(@fun, Vspan, Fsi);

% Extract individual species flows
FA = F(:, 1);
FB = F(:, 2);  % run function outside script such that is goes to flow B = 0 with changing inlet
flow rate with inital guess
FC = F(:, 3);
FD = F(:, 4);
FE = F(:, 5);
FF = F(:, 6);
FS = F(:, 7);

vol = V; %some convertor to get in kta
flows = F;
function dFdV = fun(~, F)
   FA = F(1);
   FB = F(2);
   FC = F(3);
   FD = F(4);
   FE = F(5);
   FF = F(6);
   FS = F(7);

   R = 8.314; % Gas constant  J/(mol*K)
    % in units of kPa to work with units of R

   k1f = 4.652e+13 * exp(-273000 / (R * T));
      ●     k1r = 9.91e+8 * exp(-137800 / (R * T));
   k2 = 3.85e+11 * exp(-273000 / (R * T));
   k3 = 7.083e+13 * exp(-252600 / (R * T));

   Ftot = FA + FB + FC + FD + FE + FF + FS;
   % Ftot = FA + FB + FC + FD + FE + FF;

   %R = 0.08314;
   bot = Ftot * R * T; % units of J/s or L*kPa/s
```

```
    dFAdV = -(k1f * (FA * Ptot) / bot - k1r * (FB * FC * Ptot^2) / bot^2 + 2*k2 * (FA^2 *
Ptot^2) / bot^2 + k3 * (FA * FB * Ptot^2) / bot^2);
    dFBdV = k1f * (FA * Ptot) / bot - k1r * (FB * FC * Ptot^2) / bot^2 - k3 * (FA * FB *
Ptot^2) / bot^2;
    dFCdV = k1f * (FA * Ptot) / bot - k1r * (FB * FC * Ptot^2) / bot^2;
    dFDdV = k2 * (FA^2 * Ptot^2) / bot^2;
    dFEdV = dFDdV;
    dFFdV = k3 * (FA * FB * Ptot^2) / bot^2;
    dFSdV = 0;
    dFdV = [dFAdV; dFBdV; dFCdV; dFDdV; dFEdV; dFFdV; dFSdV];
    %dFdV = [dFAdV; dFBdV; dFCdV; dFDdV; dFEdV; dFFdV];
end
end
```

Loop NPV for different graphs

```
clc; clear; close all;

% Initialize variables
R = 8.3145; % Gas constant
FA0 = 1; % Used for XA and S only, needs to be scaled
Vmax = 2000; % Maximum volume
Ptot = 200; % Operating pressure in kPa (2 bar)
T = 825 + 273.15; % Operating temperature in K
MR_values = [0.6, 0.8, 1.0]; % Steam-to-ethane molar ratio values
desiredLength = 56; % Desired length for vectors

% Prepare plot
figure;
hold on;
colors = ['b', 'r', 'g']; % Color for each MR value
legends = cell(length(MR_values), 1); % Legend for each line

for idx = 1:length(MR_values)
    MR = MR_values(idx); % Current MR value
    [V,F] = getFETi(FA0,Vmax,T,Ptot);


    FA = F(:, 1);
```

```
FB = F(:, 2);
FC = F(:, 3);
FD = F(:, 4);
FE = F(:, 5);
FF = F(:, 6);
FS = F(:, 7);

%% conversions and selectivities
XA = (FA0 - FA)/FA0;
S2 = FB ./(FA0.*XA); %for ethylene
S2 = (FB - 0)./(FA0 -FA);
S3 = FC ./((FA0).*XA); %for hydrogen
S3 = (FC - 0)./(FA0-FA);
S4 = FD ./((FA0).*XA); %for propane
S5 = S4; %for methane
S6 = FF ./((FA0).*XA); %for butane
q0 = R*T/Ptot*(1+MR);
tau = V./q0;
tau = V*Ptot./(R*T*(1+MR));
%% Recycle Flow
FAplant = 235.7./(S2.*XA); % mol/s basis
FBplant = 235.7*ones(length(FAplant),1);

RAplant = FBplant./(S2).*(1-XA)./XA;
FAplant = RAplant;
FFAplant = FBplant./S2;

FCplant = FBplant.*S3./S2;
FDplant = FBplant./2.*(1-2.*S3+S2)./S2;
FEplant = FDplant;
FFplant = FBplant.*(S3-S2)./S2;
FSplant = MR*(RAplant+FFAplant);

FFSplant = (RAplant+FFAplant)*MR;
FlowToSeparations = RAplant+FBplant+FCplant+FDplant+FEplant+FFplant+FSplant;

v =R*T*FBplant*(1+MR)./(Ptot.*S2.*XA); %volumetric flow rate
Vplant = tau.*v;
```

```
FA = RAplant;
FB = FBplant;
FC = FCplant;
FD = FDplant;
FE = FEplant;
FF = FFplant;
FS = FSplant;
FFS = FFSplant;
F = [FA, FB, FC, FD, FE, FF, FFS];
```
%%% Beginning of costing analysis

% following is getting length and diameter of reactor
%chooses middle of plant volumes

```
for i = 1:56

    Vpfr = Vplant(i)/1000;
    H_pfr = 10*(4*Vpfr/(10*pi))^(1/3)*3.28;
    dHrxn1 = 1.4*10^5; %J/mol
    dHrxn2 = -4.7*10^3; %J/mol
    dHrxn3 = -9.4*10^4; %J/mol


    D_pfr = (4*Vpfr/(10*pi))^(1/3)*3.28;
    Tsep = 200;
    F_cpfr = 2.25; % possibly missing value for Fp
    F_cfurn = 1.1+ 0.35 ; %Stainless Steel, Pyrolysis, Rated up to 500 psi
    Q_furn_rxn = FC(i)*dHrxn1 + FD(i)*dHrxn2 + FF(i)*dHrxn3;
    Q_furn_streamHeating =
75.38*FS(i)*(T-121)+136*FA(i)*(T-Tsep)+FFAplant(i)*136*(T-25);
    %Q_furn_streamHeating = 0;
    Q_furn = (Q_furn_rxn);  %J/s
    Q_furn_stream_BTU =(Q_furn_streamHeating)*(3600/1055)/1e6;
    Q_furn_BTU = (Q_furn_rxn)*(3600/1055)/1e6; %BTU/hr *10^6
    % Q_prod = (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i))*1e3; % heat
produced from burning fuel streams

    MnS = 1800; %marshall and swiss index
    PFR_cost = (MnS/280) * (101.9 *  D_pfr^1.066 * H_pfr^0.82) * (F_cpfr +2.18);  % uses
D and H for cost of PFR
    furnace_cost = (MnS/280) * (5.52e3 * Q_furn_BTU^0.85) * (F_cfurn +1.27);  %uses
```

heat duty to solve for cost of PFR furnace

furnace_cost2 = (MnS/280) * (5.52e3 * Q_furn_stream_BTU^0.85) * (F_cfurn +1.27);
% exch_cost = (Mns/280) * (101.3 * A_exch^0.65) * (F_cexch + 2.29); % uses heat
exchanger contact area for costing

% mol fracs of each species in effluent
z = F(i,:) / sum(F(i,:));

xA1 = 1; %mol frac of A in sep stream 1
xB2 = 1; %mol frac of B in sep stream 2
xC3 = FC(i)/(FC(i) + FE(i)); %mol frac of C in sep stream 3 non psa
xCpsa = 1;
xCpsa2 = .1 *FC(i)/(0.1 *FC(i)+FE(i));
xEpsa2 = FE(i)/(0.1*FC(i)+FE(i));
xD4 = FD(i)/(FD(i) + FF(i)); %mol frac of D in sep stream 4
xE3 = FE(i)/(FC(i) + FE(i)); %mol frac of E in sep stream 3 non psa
xF4 = FF(i)/(FD(i) + FF(i)); %mol frac of F in sep stream 4
xS5 = 1; %mol frac of steam in sep stream 5
%x = [xA1; xB2; xC3; xD4; xE3; xF4; xS5];

lambda = 35; % scalig factor for ideal work to real work needed for sep system
c = 0.75;

% Separation system operating expense (ISBL)

W_min_sep = (FA(i) * Tsep * R * xA1 * log(xA1/z(1)) ...
    + FB(i) * Tsep * R * xB2 * log(xB2/z(2)) ...
    + (FC(i) + FE(i)) * Tsep * R * ((xC3) * log(xC3/z(3)) + xE3 * log(xE3/z(5))) ...
    + (FD(i) + FF(i)) * Tsep * R * ((xD4) * log(xD4/z(4)) + xF4 * log(xF4/z(6))) ...
    + (FS(i)) * Tsep * R * xS5 * log(xS5/z(7)));
sep_capex = c* (lambda) * W_min_sep;
%sep_opex = lambda* 3 *W_min_sep*1e-9;
%PSA is the essentially same cost as sep syst without due to scope of project

W_min_psa =   (FA(i) * Tsep * R * xA1 * log(xA1/z(1)) ...
    + FB(i) * Tsep * R * xB2 * log(xB2/z(2)) ...
    + (0.1 * FC(i) + FE(i)) * Tsep * R * ((xCpsa2) * log(xCpsa2/z(3)) + xEpsa2 *
log(xEpsa2/z(5))) ... % 10 mol percent hydrogen in other psa stream

```
        + FC(i) * Tsep * R * xCpsa * log(xCpsa/z(3)) ...  %pure stream of hydrogen psa
        + (FD(i) + FF(i)) * Tsep * R * ((xD4) * log(xD4/z(4)) + xF4 * log(xF4/z(6))) ...
        + (FS(i)) * Tsep * R * xS5 * log(xS5/z(7)));
    psa_capex = c* lambda * W_min_psa;
    %psa_opex = lambda *3 *W_min_psa*1e-9;




    %% Net Present Value calc



    years = (0:18)';
    entpz = 0.15;
    tax = 0.27;
    dscn = (1 + entpz) .^ years;
    ISBL_nopsa = PFR_cost + furnace_cost + sep_capex+furnace_cost2; %not including heat
exchanger at this scope
    OSBL_nopsa = 0.4 * ISBL_nopsa;    %more in depth would be to find amount of
electricity used from outsource
    contingency_nopsa = (ISBL_nopsa + OSBL_nopsa) * 0.25;
    ISBL_psa = PFR_cost + furnace_cost + psa_capex+furnace_cost2; %not including heat
exchanger at this scope
    OSBL_psa = 0.4 * ISBL_psa;    %more in depth would be to find amount of electricity
used from outsource
    contingency_psa = (ISBL_psa + OSBL_psa) * 0.25;
    TFCC_nopsa = 1.3* (ISBL_nopsa + OSBL_nopsa + contingency_nopsa); %1.3 for
indirect cost
    TFCC_psa = 1.3* (ISBL_psa + OSBL_psa + contingency_psa);
    salvage = 0.05;

    %CO2_prod_cost = 125 * (3 * FD(i) + FE(i) + 4 * FF(i)) * 44.01 * 3600 * 24 * 7 * 50
/(1e+6); % [$/annum]
    CO2_prod_cost_nopsa =
125/1e9*3600*24*7*50/802*44.01*(Q_furn+Q_furn_streamHeating+lambda*W_min_sep);
    CO2_prod_cost_psa =
125/1e9*3600*24*7*50/802*44.01*(Q_furn+Q_furn_streamHeating+lambda*W_min_psa);
    ETH_stock_cost = FFAplant(i) * 200 * 30.07 * 3600 * 24 * 7 * 50 /(1e+6); % cost of
fresh ethane feed in [$/annum]
    Steam_cost = 2.38 * FFS(i) *18.02 * 3600 * 24 * 7 * 50 /(1e+6); % 2 bar and 121C steam
inlet to reactor in [$/annum]
```

NG_cost_nopsa = 3 * (1e-9) * (3600*24*7*50) * (Q_furn+Q_furn_streamHeating + lambda*W_min_sep) ;

NG_cost_psa = 3 * (1e-9) * (3600*24*7*50) * (Q_furn+Q_furn_streamHeating + lambda*W_min_psa) ; % $/mol * mol/annum .... get mol from converison down volume of rxtr

WC = 2/12 * (ETH_stock_cost+Steam_cost); % 2 months of raw materials

capex_nopsa = [1/4*TFCC_nopsa ; 1/4 * TFCC_nopsa; 1/4 * TFCC_nopsa ;1/4*TFCC_nopsa + WC;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

capex_psa= [1/4*TFCC_psa ; 1/4 * TFCC_psa; 1/4 * TFCC_psa ;1/4*TFCC_psa + WC;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

% rev_none = (900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6)) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i)));   % mol/s * KJ/mol * 3$/GJ * 1GJ/1e+6KJ   % WITHOUT PSA

% rev_psa = ((FB(i) * 28.06 * 900 + 0.9* FC(i) * 2.02 * 1400) * 3600 * 24 * 7 * 50 /(1e+6)) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (2220 * FD(i) + 802 * FE(i) + 2878 * FF(i)+ 286 * FC(i)*0.1));

rev_none = 900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6);

rev_psa = 900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6);

byprodrev_none = (3 * 3600 * 24 * 7 * 50 /(1e+6) * (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i)));

byprodrev_psa = 0.9* FC(i) * 2.02 * 1400 * 3600 * 24 * 7 * 50 /(1e+6) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (2220 * FD(i) + 802 * FE(i) + 2878 * FF(i)+ 286 * FC(i)*0.1));

revenue_none = rev_none * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1];

revenue_psa = rev_psa * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1];

% revenue_psa(19,1) = revenue_psa(19,1) + TFCC_psa*salvage;

% revenue_none(19,1) = revenue_none(19,1) + TFCC_nopsa*salvage;

REV = [revenue_none , revenue_psa]; % matrix of revenue for no psa and with psa respectively

AGS = 0.05 * REV; %gives just a vector for the payment to workers / administration

VCOP_nopsa = (CO2_prod_cost_nopsa + ETH_stock_cost + Steam_cost + NG_cost_nopsa - byprodrev_none); %variable costs of production of no psa

FCOP_nopsa = AGS(end,1); %fixed costs of operation with no psa

VCOP_psa = (CO2_prod_cost_psa + ETH_stock_cost + Steam_cost + NG_cost_psa -

byprodrev_psa); %variable costs of production with psa

        FCOP_psa = AGS(end,2); % fixed costs of production with psa

        COM_nopsa = (VCOP_nopsa + FCOP_nopsa) *
[0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1]; % energy costs and continuous raw material costs

        COM_psa = (VCOP_psa + FCOP_psa) * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1]; %
energy costs and continuous raw material costs

        GRprof_nopsa = REV(:,1) - COM_nopsa;

        GRprof_psa = REV(:,2) - COM_psa;

        cost_basis_nopsa = 21/20 * (2.28 * ISBL_nopsa);

        cost_basis_psa = 21/20 * (2.28 * ISBL_psa);

        depriciation_nopsa = cost_basis_nopsa *
[0;0;0;0;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0;0;0;0;0]; %ten year linear dpereiciation model

        depriciation_psa = cost_basis_psa *
[0;0;0;0;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0;0;0;0;0]; %ten year linear dpereiciation model

        tax_inc_nopsa = GRprof_nopsa - depriciation_nopsa;

        tax_inc_psa = GRprof_psa - depriciation_psa;

        tax_paid_nopsa = tax * tax_inc_nopsa;

        tax_paid_psa = tax * tax_inc_psa;

        CashFlow_nopsa = (REV(:,1) - COM_nopsa - depriciation_nopsa) .* (1 - tax) -
capex_nopsa + depriciation_nopsa;

        CashFlow_psa = (REV(:,2) - COM_psa - depriciation_psa) .* (1 - tax) - capex_psa +
depriciation_psa;

        CashFlow_nopsa(19,1) = CashFlow_nopsa(19,1) - TFCC_nopsa*salvage;

        CashFlow_psa(19,1) = CashFlow_psa(19,1) - TFCC_psa*salvage;

        PV_nopsa = CashFlow_nopsa ./ dscn;

        PV_psa = CashFlow_psa./dscn;

        NPV_nopsa = zeros(19,1);

        NPV_psa = zeros(19,1);

        for j = 2:length(years)

          NPV_nopsa(1) = PV_nopsa(1);

          NPV_nopsa(j) = PV_nopsa(j) + NPV_nopsa(j-1);

          NPV_psa(1) = PV_psa(1);

          NPV_psa(j) = PV_psa(j) + NPV_psa(j-1);

```
            end

        NV = zeros(19,1);

        for j = 1:length(years)
            NV_nopsa(j) = sum(CashFlow_nopsa,1:j);
            NV_psa(j) = sum(CashFlow_psa,1:j);
        end



        % CFD_none = table(years, capex, REV(:,n), COM, GRprof, depriciation, tax_inc,
tax_paid, CashFLow, PV, NPV, NV, ...
        %     'VariableNames', ['Years', 'Rev', 'COM', 'GRprof', 'Dep', 'Taxable Inc', 'Taxes Paid',
'Cash Flow', 'PV', 'NPV', 'NV'])
        CFD_none = table(years, capex_nopsa, REV(:,1), COM_nopsa, GRprof_nopsa,
depriciation_nopsa, tax_inc_nopsa, tax_paid_nopsa, CashFlow_nopsa, PV_nopsa,
NPV_nopsa, NV_nopsa');
        Money_No(i) = CFD_none{19,"NPV_nopsa"};

        % CFD_PSA = table(years, capex, REV(:,n), COM, GRprof, depriciation, tax_inc,
tax_paid, CashFLow, PV, NPV, NV, ...
        %     'VariableNames', ['Years', 'Rev', 'COM', 'GRprof', 'Dep', 'Taxable Inc', 'Taxes Paid',
'Cash Flow', 'PV', 'NPV', 'NV'])
        CFD_PSA = table(years, capex_psa, REV(:,2), COM_psa, GRprof_psa,
depriciation_psa, tax_inc_psa, tax_paid_psa, CashFlow_psa, PV_psa, NPV_psa, NV_psa');
        Money_PSA(i) = CFD_PSA{19,"NPV_psa"};



    end

  % Ensure Vplant and Money_PSA are of length 56
currentLength = length(Vplant);
if currentLength > desiredLength
    Vplant = Vplant(1:desiredLength);
    Money_PSA = Money_PSA(1:desiredLength);
elseif currentLength < desiredLength
    originalIndices = linspace(1, currentLength, currentLength);
    targetIndices = linspace(1, currentLength, desiredLength);
    Vplant = interp1(originalIndices, Vplant, targetIndices, 'linear', 'extrap');
```

```matlab
    Money_PSA = interp1(originalIndices, Money_PSA, targetIndices, 'linear', 'extrap');
  end


  plot(Vplant/1e3, Money_PSA/1e6, colors(idx), 'LineWidth', 2);
  legends{idx} = ['MR = ' num2str(MR_values(idx))];
end

xlim([0 100]);
ylim([0 160]);
xlabel('Reactor Volume [m^3]', 'FontWeight', 'bold');
ylabel('Net Present Value [$MM/annum]', 'FontWeight', 'bold');
legend(legends, 'Location', 'Best');
box off; % Removes top and right borders
set(gca, 'FontWeight', 'bold'); % Makes the axis bold
hold off;
```

NPV Optimization

```matlab
%give a V, T, Ptot to get a FA_sol...from this FA_sol, optimize NPV with it
clc; clear; close all;
T = 825+273.15;
Ptot = 200;
R = 8.3145;
MR = 0.6;


%% Species Flows
FA0 = 1; %Used for XA and S only, needs to be scaled
Vmax = 2000;
[V,F] = getFETi(FA0,Vmax,T,Ptot);


FA = F(:, 1);
FB = F(:, 2);
FC = F(:, 3);
FD = F(:, 4);
FE = F(:, 5);
FF = F(:, 6);
FS = F(:, 7);
```

```matlab
%% conversions and selectivities
XA = (FA0 - FA)/FA0;
S2 = FB ./(FA0.*XA); %for ethylene
S2 = (FB - 0)./(FA0 -FA);
S3 = FC ./((FA0).*XA); %for hydrogen
S3 = (FC - 0)./(FA0-FA);
S4 = FD ./((FA0).*XA); %for propane
S5 = S4; %for methane
S6 = FF ./((FA0).*XA); %for butane
q0 = R*T/Ptot*(1+MR);
tau = V./q0;
tau = V*Ptot./(R*T*(1+MR));
%% Recycle Flow
FAplant = 235.7./(S2.*XA); % mol/s basis
FBplant = 235.7*ones(length(FAplant),1);

RAplant = FBplant./(S2).*(1-XA)./XA;
FAplant = RAplant;
FFAplant = FBplant./S2;

FCplant = FBplant.*S3./S2;
FDplant = FBplant./2.*(1-2.*S3+S2)./S2;
FEplant = FDplant;
FFplant = FBplant.*(S3-S2)./S2;
FSplant = MR*(RAplant+FFAplant);

FFSplant = (RAplant+FFAplant)*MR;
FlowToSeparations = RAplant+FBplant+FCplant+FDplant+FEplant+FFplant+FSplant;

v =R*T*FBplant*(1+MR)./(Ptot.*S2.*XA); %volumetric flow rate
Vplant = tau.*v;
% conclusion draft?,
% the conceptualized steam ethane cracker ascends as a luminary of industrial sorcery,
% fated to bestow an unparalleled bounty of 200 kta of the most exquisitely refined
% polymer-grade ethylene, thus inscribing a formidable saga of prosperity
% and an unwavering fealty to the principles of carbon neutrality across the
% ever-morphing ether of the chemical market cosmos.

% Economic oracles foretell an enthralling net present value (NPV) of $140 million,
% bolstered by a substantial total capital investment (TCI) of $168 million and an
```

```matlab
% internal rate of return (IRR) that boasts a resplendent 28%, crafting a portrait of
% robust profitability and compelling investment allure that is both sumptuous and magnetic.
FA = RAplant;
FB = FBplant;
FC = FCplant;
FD = FDplant;
FE = FEplant;
FF = FFplant;
FS = FSplant;
FFS = FFSplant;
F = [FA, FB, FC, FD, FE, FF, FFS];
%% Beginning of costing analysis

% following is getting length and diameter of reactor
%chooses middle of plant volumes

for i = 1:70

    Vpfr = Vplant(i)/1000;
    H_pfr = 10*(4*Vpfr/(10*pi))^(1/3)*3.28;
    dHrxn1 = 1.4*10^5; %J/mol
    dHrxn2 = -4.7*10^3; %J/mol
    dHrxn3 = -9.4*10^4; %J/mol


    D_pfr = (4*Vpfr/(10*pi))^(1/3)*3.28;
    Tsep = 200;
    F_cpfr = 2.25; % possibly missing value for Fp
    F_cfurn = 1.1+ 0.35 ; %Stainless Steel, Pyrolysis, Rated up to 500 psi
    Q_furn_rxn = FC(i)*dHrxn1 + FD(i)*dHrxn2 + FF(i)*dHrxn3;
    Q_furn_streamHeating =
75.38*FS(i)*(T-121)+136*FA(i)*(T-Tsep)+FFAplant(i)*136*(T-25);
    %Q_furn_streamHeating = 0;
    Q_furn = (Q_furn_rxn);  %J/s
    Q_furn_stream_BTU =(Q_furn_streamHeating)*(3600/1055)/1e6;
    Q_furn_BTU = (Q_furn_rxn)*(3600/1055)/1e6; %BTU/hr *10^6
    % Q_prod = (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i))*1e3; % heat
produced from burning fuel streams

    MnS = 1800; %marshall and swiss index
    PFR_cost = (MnS/280) * (101.9 *  D_pfr^1.066 * H_pfr^0.82) * (F_cpfr +2.18);  % uses D
```

and H for cost of PFR

    furnace_cost = (MnS/280) * (5.52e3 * Q_furn_BTU^0.85) * (F_cfurn +1.27); %uses heat duty to solve for cost of PFR furnace

    furnace_cost2 = (MnS/280) * (5.52e3 * Q_furn_stream_BTU^0.85) * (F_cfurn +1.27);

    % exch_cost = (Mns/280) * (101.3 * A_exch^0.65) * (F_cexch + 2.29); % uses heat exchanger contact area for costing

    % mol fracs of each species in effluent

    z = F(i,:) / sum(F(i,:));

    xA1 = 1; %mol frac of A in sep stream 1

    xB2 = 1; %mol frac of B in sep stream 2

    xC3 = FC(i)/(FC(i) + FE(i)); %mol frac of C in sep stream 3 non psa

    xCpsa = 1;

    xCpsa2 = .1 *FC(i)/(0.1 *FC(i)+FE(i));

    xEpsa2 = FE(i)/(0.1*FC(i)+FE(i));

    xD4 = FD(i)/(FD(i) + FF(i)); %mol frac of D in sep stream 4

    xE3 = FE(i)/(FC(i) + FE(i)); %mol frac of E in sep stream 3 non psa

    xF4 = FF(i)/(FD(i) + FF(i)); %mol frac of F in sep stream 4

    xS5 = 1; %mol frac of steam in sep stream 5

    %x = [xA1; xB2; xC3; xD4; xE3; xF4; xS5];

    lambda = 35; % scalig factor for ideal work to real work needed for sep system

    c = 0.75;

    % Separation system operating expense (ISBL)

    W_min_sep = (FA(i) * Tsep * R * xA1 * log(xA1/z(1))) ...

      + FB(i) * Tsep * R * xB2 * log(xB2/z(2)) ...

      + (FC(i) + FE(i)) * Tsep * R * ((xC3) * log(xC3/z(3)) + xE3 * log(xE3/z(5))) ...

      + (FD(i) + FF(i)) * Tsep * R * ((xD4) * log(xD4/z(4)) + xF4 * log(xF4/z(6))) ...

      + (FS(i)) * Tsep * R * xS5 * log(xS5/z(7)));

    sep_capex = c* (lambda) * W_min_sep;

    %sep_opex = lambda* 3 *W_min_sep*1e-9;

    %PSA is the essentially same cost as sep syst without due to scope of project

    W_min_psa =   (FA(i) * Tsep * R * xA1 * log(xA1/z(1))) ...

      + FB(i) * Tsep * R * xB2 * log(xB2/z(2)) ...

```
    + (0.1 * FC(i) + FE(i)) * Tsep * R * ((xCpsa2) * log(xCpsa2/z(3)) + xEpsa2 *
log(xEpsa2/z(5))) ...  % 10 mol percent hydrogen in other psa stream
    + FC(i) * Tsep * R * xCpsa * log(xCpsa/z(3)) ...  %pure stream of hydrogen psa
    + (FD(i) + FF(i)) * Tsep * R * ((xD4) * log(xD4/z(4)) + xF4 * log(xF4/z(6))) ...
    + (FS(i)) * Tsep * R * xS5 * log(xS5/z(7)));
  psa_capex = c* lambda * W_min_psa;
  %psa_opex = lambda *3 *W_min_psa*1e-9;
```

%% Net Present Value calc

```
  years = (0:18)';
  entpz = 0.15;
  tax = 0.27;
  dscn = (1 + entpz) .^ years;
  ISBL_nopsa = PFR_cost + furnace_cost + sep_capex+furnace_cost2; %not including heat
exchanger at this scope
  OSBL_nopsa = 0.4 * ISBL_nopsa;    %more in depth would be to find amount of electricity
used from outsource
  contingency_nopsa = (ISBL_nopsa + OSBL_nopsa) * 0.25;
  ISBL_psa = PFR_cost + furnace_cost + psa_capex+furnace_cost2; %not including heat
exchanger at this scope
  OSBL_psa = 0.4 * ISBL_psa;    %more in depth would be to find amount of electricity used
from outsource
  contingency_psa = (ISBL_psa + OSBL_psa) * 0.25;
  TFCC_nopsa = 1.3* (ISBL_nopsa + OSBL_nopsa + contingency_nopsa); %1.3 for indirect
cost
  TFCC_psa = 1.3* (ISBL_psa + OSBL_psa + contingency_psa);
  salvage = 0.05;

  %CO2_prod_cost = 125 * (3 * FD(i) + FE(i) + 4 * FF(i)) * 44.01 * 3600 * 24 * 7 * 50
/(1e+6); % [$/annum]
  CO2_prod_cost_nopsa =
125/1e9*3600*24*7*50/802*44.01*(Q_furn+Q_furn_streamHeating+lambda*W_min_sep);
  CO2_prod_cost_psa =
125/1e9*3600*24*7*50/802*44.01*(Q_furn+Q_furn_streamHeating+lambda*W_min_psa);
  ETH_stock_cost = FFAplant(i) * 200 * 30.07 * 3600 * 24 * 7 * 50 /(1e+6); % cost of fresh
ethane feed in [$/annum]
```

Steam_cost = 2.38 * FFS(i) *18.02 * 3600 * 24 * 7 * 50 /(1e+6); % 2 bar and 121C steam inlet to reactor in [$/annum]

NG_cost_nopsa = 3 * (1e-9) * (3600*24*7*50) * (Q_furn+Q_furn_streamHeating + lambda*W_min_sep) ;

NG_cost_psa = 3 * (1e-9) * (3600*24*7*50) * (Q_furn+Q_furn_streamHeating + lambda*W_min_psa) ; % $/mol * mol/annum .... get mol from converison down volume of rxtr

WC = 2/12 * (ETH_stock_cost+Steam_cost); % 2 months of raw materials

capex_nopsa = [1/4*TFCC_nopsa ; 1/4 * TFCC_nopsa; 1/4 * TFCC_nopsa ;1/4*TFCC_nopsa + WC;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

capex_psa= [1/4*TFCC_psa ; 1/4 * TFCC_psa; 1/4 * TFCC_psa ;1/4*TFCC_psa + WC;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

% rev_none = (900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6)) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i)));   % mol/s * KJ/mol * 3$/GJ * 1GJ/1e+6KJ   % WITHOUT PSA

% rev_psa = ((FB(i) * 28.06 * 900 + 0.9* FC(i) * 2.02 * 1400) * 3600 * 24 * 7 * 50 /(1e+6)) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (2220 * FD(i) + 802 * FE(i) + 2878 * FF(i)+ 286 * FC(i)*0.1));

rev_none = 900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6);

rev_psa = 900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6);

byprodrev_none = (3 * 3600 * 24 * 7 * 50 /(1e+6) * (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i)));

byprodrev_psa = 0.9* FC(i) * 2.02 * 1400 * 3600 * 24 * 7 * 50 /(1e+6) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (2220 * FD(i) + 802 * FE(i) + 2878 * FF(i)+ 286 * FC(i)*0.1));

revenue_none = rev_none * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1];

revenue_psa = rev_psa * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1];

% revenue_psa(19,1) = revenue_psa(19,1) + TFCC_psa*salvage;

% revenue_none(19,1) = revenue_none(19,1) + TFCC_nopsa*salvage;

REV = [revenue_none , revenue_psa]; % matrix of revenue for no psa and with psa respectively

AGS = 0.05 * REV; %gives just a vector for the payment to workers / administration

VCOP_nopsa = (CO2_prod_cost_nopsa + ETH_stock_cost + Steam_cost + NG_cost_nopsa - byprodrev_none); %variable costs of production of no psa

```
FCOP_nopsa = AGS(end,1); %fixed costs of operation with no psa
VCOP_psa = (CO2_prod_cost_psa + ETH_stock_cost + Steam_cost + NG_cost_psa -
byprodrev_psa); %variable costs of production with psa
FCOP_psa = AGS(end,2); % fixed costs of production with psa
COM_nopsa = (VCOP_nopsa + FCOP_nopsa) * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1];
% energy costs and continuous raw material costs
COM_psa = (VCOP_psa + FCOP_psa) * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1]; %
energy costs and continuous raw material costs

GRprof_nopsa = REV(:,1) - COM_nopsa;
GRprof_psa = REV(:,2) - COM_psa;

cost_basis_nopsa = 21/20 * (2.28 * ISBL_nopsa);
cost_basis_psa = 21/20 * (2.28 * ISBL_psa);

depriciation_nopsa = cost_basis_nopsa *
[0;0;0;0;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0;0;0;0;0]; %ten year linear dpereiciation model
depriciation_psa = cost_basis_psa *
[0;0;0;0;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0;0;0;0;0]; %ten year linear dpereiciation model

tax_inc_nopsa = GRprof_nopsa - depriciation_nopsa;
tax_inc_psa = GRprof_psa - depriciation_psa;

tax_paid_nopsa = tax * tax_inc_nopsa;
tax_paid_psa = tax * tax_inc_psa;
CashFlow_nopsa = (REV(:,1) - COM_nopsa - depriciation_nopsa) .* (1 - tax) -
capex_nopsa + depriciation_nopsa;
CashFlow_psa = (REV(:,2) - COM_psa - depriciation_psa) .* (1 - tax) - capex_psa +
depriciation_psa;
CashFlow_nopsa(19,1) = CashFlow_nopsa(19,1) - TFCC_nopsa*salvage;
CashFlow_psa(19,1) = CashFlow_psa(19,1) - TFCC_psa*salvage;
PV_nopsa = CashFlow_nopsa ./ dscn;
PV_psa = CashFlow_psa./dscn;
NPV_nopsa = zeros(19,1);
NPV_psa = zeros(19,1);


for j = 2:length(years)
    NPV_nopsa(1) = PV_nopsa(1);
    NPV_nopsa(j) = PV_nopsa(j) + NPV_nopsa(j-1);
```

```matlab
        NPV_psa(1) = PV_psa(1);
        NPV_psa(j) = PV_psa(j) + NPV_psa(j-1);
    end

    NV = zeros(19,1);

    for j = 1:length(years)
        NV_nopsa(j) = sum(CashFlow_nopsa,1:j);
        NV_psa(j) = sum(CashFlow_psa,1:j);
    end



    % CFD_none = table(years, capex, REV(:,n), COM, GRprof, depriciation, tax_inc,
tax_paid, CashFLow, PV, NPV, NV, ...
    %    'VariableNames', ['Years', 'Rev', 'COM', 'GRprof', 'Dep', 'Taxable Inc', 'Taxes Paid',
'Cash Flow', 'PV', 'NPV', 'NV'])
    CFD_none = table(years, capex_nopsa, REV(:,1), COM_nopsa, GRprof_nopsa,
depriciation_nopsa, tax_inc_nopsa, tax_paid_nopsa, CashFlow_nopsa, PV_nopsa,
NPV_nopsa, NV_nopsa');
    Money_No(i) = CFD_none{19,"NPV_nopsa"};

    % CFD_PSA = table(years, capex, REV(:,n), COM, GRprof, depriciation, tax_inc,
tax_paid, CashFLow, PV, NPV, NV, ...
    %    'VariableNames', ['Years', 'Rev', 'COM', 'GRprof', 'Dep', 'Taxable Inc', 'Taxes Paid',
'Cash Flow', 'PV', 'NPV', 'NV'])
    CFD_PSA = table(years, capex_psa, REV(:,2), COM_psa, GRprof_psa, depriciation_psa,
tax_inc_psa, tax_paid_psa, CashFlow_psa, PV_psa, NPV_psa, NV_psa');
    Money_PSA(i) = CFD_PSA{19,"NPV_psa"};



end

% figure(1)
% plot(XA,Money_PSA/1e6,'g','LineWidth',2)
% ylim([0 5e2])
% xlabel('Single pass conversion')
% ylabel('Net Present Value $MM/annum')
% figure(2)
% plot(Vplant/1e3,Money_PSA/1e6,'k','LineWidth',2)
```

```matlab
% ylim([0 5e2])
% xlabel('Reactor Volume [m^3]')
% ylabel('Net Present Value $MM/annum')
[x,y_psa] = max(Money_PSA);
sprintf('Max NPV PSA $MM/annum:  %0.5g',x/1e6)
sprintf('Reactor Volume m^3 : %0.5g',Vplant(y_psa)/1e3)
[x,y] = max(Money_No);
sprintf('Max NPV No PSA $MM/annum:  %0.5g',x/1e6)
sprintf('Reactor Volume m^3 : %0.5g',Vplant(y)/1e3)


%%% Sensitivity Analysis

figure(1)

plot(Vplant/1e3, Money_PSA/1e6, 'b-', 'LineWidth', 2);
xlim([0 100])
ylim([0 160])
xlabel('Reactor Volume [m^3]', 'FontWeight', 'bold');
ylabel('Net Present Value [$MM/annum]', 'FontWeight', 'bold');
title('');
box off; % Removes top and right borders
set(gca, 'FontWeight', 'bold'); % Makes the axis bolded
```

New NPV Code

```matlab
%give a V, T, Ptot to get a FA_sol...from this FA_sol, optimize NPV with it
clc; clear; close all;
T = 825+273.15;
Ptot = 200;
R = 8.3145;
MR = 0.6;

%%% Species Flows
FA0 = 1; %Used for XA and S only, needs to be scaled
Vmax = 2000;
[V,F] = getFETi(FA0,Vmax,T,Ptot);


FA = F(:, 1);
FB = F(:, 2);
```

```matlab
FC = F(:, 3);
FD = F(:, 4);
FE = F(:, 5);
FF = F(:, 6);
FS = F(:, 7);

%% conversions and selectivities
XA = (FA0 - FA)/FA0;
S2 = FB ./(FA0.*XA); %for ethylene
S2 = (FB - 0)./(FA0 -FA);
S3 = FC ./((FA0).*XA); %for hydrogen
S3 = (FC - 0)./(FA0-FA);
S4 = FD ./((FA0).*XA); %for propane
S5 = S4; %for methane
S6 = FF ./((FA0).*XA); %for butane
q0 = R*T/Ptot*(1+MR);
tau = V./q0;
tau = V*Ptot./(R*T*(1+MR));
%% Recycle Flow
FAplant = 235.7./(S2.*XA); % mol/s basis
FBplant = 235.7*ones(length(FAplant),1);

RAplant = FBplant./(S2).*(1-XA)./XA;
FAplant = RAplant;
FFAplant = FBplant./S2;

FCplant = FBplant.*S3./S2;
FDplant = FBplant./2.*(1-2.*S3+S2)./S2;
FEplant = FDplant;
FFplant = FBplant.*(S3-S2)./S2;
FSplant = MR*(RAplant+FFAplant);

FFSplant = (RAplant+FFAplant)*MR;
FlowToSeparations = RAplant+FBplant+FCplant+FDplant+FEplant+FFplant+FSplant;

v =R*T*FBplant*(1+MR)./(Ptot.*S2.*XA); %volumetric flow rate
Vplant = tau.*v;

% FS_postflash = 9.3713;
FA = RAplant;
FB = FBplant;
FC = FCplant;
FD = FDplant;
FE = FEplant;
FF = FFplant;
FS = FSplant;
```

```
FFS = FFSplant;
F = [FA, FB, FC, FD, FE, FF, FFS];
%% Beginning of costing analysis

% following is getting length and diameter of reactor
%chooses middle of plant volumes

for i = 1:36

    Vpfr = 16.6;
    H_pfr = 10*(4*Vpfr/(10*pi))^(1/3)*3.28;
    dHrxn1 = 1.4*10^5; %J/mol
    dHrxn2 = -4.7*10^3; %J/mol
    dHrxn3 = -9.4*10^4; %J/mol
    MnS = 1800; %marshall and swiss index
    elek_cost = 0.04 / 3.6e6; % $/kWh * kWh/J

    D_pfr = (4*Vpfr/(10*pi))^(1/3)*3.28;

    Tsep_water = 278; % CHANGE BASED ON WHAT THE PSA FOR REMOVING WATER
ENDS UP BEING
    Tsep_H2 = 273+9; % the h2 psa sep temp
    F_cpfr = 2.25; % possibly missing value for Fp


    Q_furn_rxn = FC(i)*dHrxn1 + FD(i)*dHrxn2 + FF(i)*dHrxn3;
    Q_furn_rxn = 3.623e7;

    Q_furn1 = 3.781e6; % 200 kPa   E-100
    Q_furn2 = 795.5e3; % 6000 kPa   E-111
    Q_furn3 = 0; % 6000 kPa   E-107
    Q_furn4 = 1.169e7; % 2200 kPa... this is a reboiler   dist1
    Q_furn5 = 3086e3; % 2200 kPa...also a reboiler    dist2
    Q_furn6 = 409.9e3; % E-110 heater

    Q_furn_streamHeating = Q_furn1 + Q_furn2 + Q_furn3 + Q_furn4 + Q_furn5 + Q_furn6;
%all the heating done across the plant including reboilers, exempt of reactor
    %Q_furn_streamHeating = 0;

    % J/s all the cooling streams energy duty
    Q_cool1 = 1.168e7;  % E-101 weak cooling, cools stream to
    Q_cool2 = 2760000;  % Cond dist 2 weak cooling, condensor in dist not costed here
    Q_cool3 = 2538000; % E-108 mid cooling, cools stream from
    Q_cool4 = 1.162E7;% Cond dist 1 mid cooling, condensor not costed here
    Q_cool5 = 8199000; % E-103 strong cooling, cools stream from
```

```
Q_coolers_streams = [Q_cool1, Q_cool2, Q_cool3, Q_cool4, Q_cool5];
Q_coolers_Temps = [-5,-25, -35, -43, -141];
% [-5,-25, -35, -43, -141]
% Q_coolers_Temps = [-5,-5, -5, -5, -5];
Q_cooler_streamCooling = sum(Q_coolers_streams);

Q_furn = (Q_furn_rxn);  %J/s
```

Q_furn_stream_BTU =(Q_furn_streamHeating)*(3600/1055)/1e6; %BTU/hr e+6 , this stuff is just for costing the equipment

```
Q_furn_BTU = (Q_furn_rxn)*(3600/1055)/1e6; %BTU/hr *10^6

Q_coolers_BTU = Q_cooler_streamCooling * (3600/1055)/1e6;
% Q_prod = (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i))*1e3; % heat
```
produced from burning fuel streams

```
%% heat exchanger costing
Tlm = 30;

F_dhex = 1;
F_phex = 0; F_phex300 = 0.1; F_phex400 = 0.25; F_phex800 = 0.52; F_phex1000 = 0.55;
F_mhex = 3.75;
Fc_hex = (F_dhex + F_phex) * F_mhex;
Fc_hex1000 = (F_dhex + F_phex1000) * F_mhex;
kjh_W = 0.28;

% these are in kJ/hr
Q_hex1 = 1.226e8; % E-102
Q_hex2 = 7.147e6; % E-105
Q_hex3 = 7.885e6; % heat ex 2
Q_hex4 = 4.289e6; % E-109
% Q_hex5 = ; % E-110
Q_hex6 = 7.651e6; % E-106
Q_hex7 = 9.918e5; % E-104


duty_hex1 = Q_hex1/9 * ones(1,9);
% duty_hex1 = Q_hex1/8.7791 * ones(1,9);
% duty_hex1(9) = Q_hex1/8.7791 * 0.7791;
Tlm1 = 72.14; %Hysys
A_hex1 = duty_hex1.*kjh_W / (55 * Tlm1) *10.76 ; % E-102 200kpa
A_hex1 = Q_hex1/3.6/55/Tlm1*3.28^2; %ft^2
A_hex1 = 25000; %area for one hx is larger than 25k ft^2, set to max
n_he_1 = Q_hex1/3.6/(55*Tlm1*A_hex1/3.28^2);
hex1_capex = ceil(n_he_1)*(MnS/280)* 101.3 * A_hex1.^ 0.65 * (2.29 + Fc_hex);
```

```
Tlm2 = 59.57;
%A_hex2 = Q_hex2*kjh_W / (55 * Tlm) *10.76; % E-105 200kpa
%A_hex2 = Q_hex2/3.6/55/Tlm2*3.28^2;
A_hex2 = 25000*.2608;
n_he_2 = Q_hex2/3.6/(55*Tlm2*A_hex2/3.28^2);
hex2_capex = n_he_2*(MnS/280)* 101.3 * A_hex2 ^ 0.65 * (2.29 + Fc_hex);

Tlm3= 78.84;
%A_hex3 =  Q_hex3*kjh_W / (55 * Tlm) *10.76; % heat ex 2 200kpa
A_hex3 = 25000*.126;
n_he_3 = Q_hex3/3.6/(95*Tlm3*A_hex3/3.28^2);
hex3_capex = (MnS/280)* 101.3 * A_hex3 ^ 0.65 * (2.29 + Fc_hex);

Tlm4 = 101;
%A_hex4 =  Q_hex4*kjh_W/ (55 * 107) *10.76; % E-109 200kpa
A_hex4 = 25000*0.0534;
n_he_4 = Q_hex4/3.6/(95*Tlm4*A_hex4/3.28^2);
hex4_capex = (MnS/280)* 101.3 * A_hex4 ^ 0.65 * (2.29 + Fc_hex);

% A_hex5 = Q_hex5*kjh_W/ (55 * Tlm) *10.76; % E-110 200kpa
% hex5_capex = (MnS/280)* 101.3 * A_hex5 ^ 0.65 * (2.29 + Fc_hex);
Tlm6 =88;
%A_hex6 = Q_hex6*kjh_W/ (55 * 90) *10.76; % E-106 6000kpa
A_hex6 = 25000*0.1094;
n_he_6 = Q_hex6/3.6/(95*Tlm6*A_hex6/3.28^2);
hex6_capex = (MnS/280)* 101.3 * A_hex6 ^ 0.65 * (2.29 + Fc_hex1000);

Tlm7 = 50;
%A_hex7 = Q_hex7*kjh_W/ (55 * 50) *10.76; % E-104 6000kpa
A_hex7 = 25000*0.0250;
n_he_7 = Q_hex7/3.6/(95*Tlm7*A_hex7/3.28^2);
hex7_capex = (MnS/280)* 101.3 * A_hex7 ^ 0.65 * (2.29 + Fc_hex1000);



   heat_ex_CAPEX = hex1_capex + hex2_capex + hex3_capex + hex4_capex + hex6_capex + hex7_capex;

   %% furnace costing

   F_cfurn = 1.1+ 0.35 ; %Chrome Steel, Pyrolysis, Rated up to 500 psi
   PFR_cost = (MnS/280) * (101.9 *  D_pfr^1.066 * H_pfr^0.82) * (F_cpfr +2.18);  % uses D
and H for cost of PFR
   furnace_cost = (MnS/280) * (5.52e3 * Q_furn_BTU^0.85) * (F_cfurn +1.27);  %uses heat
duty to solve for cost of PFR furnace
```

```
F_cfurn1 = 1.45;
F_cfurn2 = 1.6;
F_cfurn3 = 1.6;

furnace_cost1 = (MnS/280) * (5.07e3 * (Q_furn1*(3600/1055)/1e6)^0.85) * (F_cfurn1
+1.23);
furnace_cost2 = (MnS/280) * (5.07e3 * (Q_furn2*(3600/1055)/1e6)^0.85) * (F_cfurn2
+1.23);
furnace_cost3 = (MnS/280) * (5.07e3 * (Q_furn3*(3600/1055)/1e6)^0.85) * (F_cfurn3
+1.23);

furnace_tot_cost = furnace_cost + furnace_cost1 + furnace_cost2 + furnace_cost3;


% mol fracs of each species in effluent
FS_postflash = 9.3713;
z = F(i,:) / (sum(F(i,:))) ; % <---- ENTER THE ACTUAL MOLAR FLOW RATE OF
STEAM AFTER THE FLASH REMOVAL
strm1 = 2272/3.6;
xA1 = FA(i) / strm1;
xB1 = FB(i) / strm1;
xC1 = FC(i) / strm1;
xD1 = FD(i) / strm1;
xE1 = FE(i) / strm1;
xF1 = FF(i) / strm1;
xS2 = 1;

lambda = 35; % scalig factor for ideal work to real work needed for sep system
c = 0.75;

%% Cooler exchangers costing

F_dcoolex = 1;
F_pcoolex = 0; F_pcoolex300 = 0.1; F_pcoolex400 = 0.25; F_pcoolex800 = 0.52;
F_pcoolex1000 = 0.55;
F_mcoolex = 3.75;
Fc_coolex = (F_dcoolex + F_pcoolex) * F_mcoolex;
Fc_coolex3 = (F_dcoolex + F_pcoolex300) * F_mcoolex;



% duty_coolex1 = Q_cool1/27 * ones(1,27);
% duty_coolex1 = Q_cool1/26.5346 * ones(1,27);
% duty_coolex1(27) = Q_cool1/26.5346 * 0.5346;
```

```matlab
% A_coolex1 = duty_coolex1 .* 0.28/55*10.76 ; % E-101   200kpa
  A_coolex1 = 25000;
  n_cool_1 = Q_cool1/(55*Tlm*A_coolex1/3.28^2);
% coolex_capex1 = sum((MnS/280)* 101.3 * A_coolex1.^ 0.65 * (2.29 + Fc_coolex));
  coolex_capex1 = ceil(n_cool_1)* (MnS/280)* 101.3 * A_coolex1.^ 0.65 * (2.29 +
Fc_coolex);


  duty_coolex2 = Q_cool5/19 * ones(1,19);
% duty_coolex2 = Q_cool5/18.3573 * ones(1,19);
% duty_coolex2(19) = Q_cool5/18.3573 * 0.3573;
  A_coolex2 = duty_coolex2 .* 0.28/55*10.76 ; % E-103    200kpa
  A_coolex2 = 25000*.6623;
  n_cool_2 = Q_cool3/(55*Tlm*A_coolex2/3.28^2);
%coolex_capex2 = sum((MnS/280)* 101.3 * A_coolex2.^ 0.65 * (2.29 + Fc_coolex));
  coolex_capex2 =  ceil(n_cool_2)*(MnS/280)* 101.3 * A_coolex2.^ 0.65 * (2.29 +
Fc_coolex);


  duty_coolex3 = Q_cool3/6 * ones(1,6);
% duty_coolex3 = Q_cool3/4.9498 * ones(1,5);
% duty_coolex3(5) = Q_cool3/4.9498 * 0.9498;
  A_coolex3 =  duty_coolex3 .* 0.28/55*10.76 ; % E-108 1600kpa
  A_coolex3 = 25000*.3972;
  n_cool_3 = Q_cool3/(55*50*A_coolex3/3.28^2);
  coolex_capex3 = ceil(n_cool_3)*(MnS/280)* 101.3 * A_coolex3 .^ 0.65 * (2.29 +
Fc_coolex3);



  cool_ex_CAPEX = coolex_capex1 + coolex_capex2 + coolex_capex3;



%% Separation system operating expense (ISBL)

%% expander costing

  expander_CAPEX = 0;
  expander_OPEX = elek_cost * 3.024e7 * 898800; % negative operating cost since we can
take away from utilities, PUT AS A NEGATIVE UTILITIES

%% compressor costings, including pumps

  compressor_OPEX = elek_cost * 1057100 * 3.024e7 ; % electricity cost times the required
duty to get the $/annum $/J * J/s * s/annum
%% flash costing (one for water and one for hydrogen)
```

D_fh2o = 3.2 * 3.28; % diameters and heights for these towers are in feet
H_fh2o = 11.2 * 3.28;
F_m_fh2o = 2.25;
F_p_fh2o = 1;
F_cfh2o = F_m_fh2o * F_p_fh2o;
flash_h2o_CAPEX = (MnS/280) * 101.9 * D_fh2o^1.066 * H_fh2o^0.82 *(2.18 + F_cfh2o);
% flash_h2o_OPEX = ; % this operating expense will be the energy cost for the cooler right before the flashes

D_fH2 = 1.372 * 3.28;
H_fH2 = 7.544 * 3.28;
F_m_fH2 = 2.25;
F_p_fH2 = 1;
F_cfH2 = F_m_fH2 * F_p_fH2;
flash_H2_CAPEX1 = (MnS/280) * 101.9 * D_fH2^1.066 * H_fH2^0.82 *(2.18 + F_cfH2);
% flash_H2_OPEX1 = ; % as well this is an energy cost for the cooler right before the

% NO THIRD FLASH FOR THIS SCHEME
% D_fhH2_2 = 1.524 * 3.28;
% H_fH2_2 = 5.334 * 3.28;
% F_m_fH2_2 = 2.25;
% F_p_fH2_2 = 1;
% F_cfH2_2 = F_m_fH2_2 * F_p_fH2_2;
% flash_H2_CAPEX2 = (MnS/280) * 101.9 * D_fH2^1.066 * H_fH2^0.82 *(2.18 + F_cfH2);
% % flash_H2_OPEX_2 = ; % as well this is an energy cost for the cooler right before the

flash_CAPEX = flash_H2_CAPEX1 + flash_h2o_CAPEX;

%% Distillation costing (split C2= from C2 and C4) (split the C2 and C4)
MnS = 1800;

D_dist1 = 1.5 * 3.281;
H_dist1 = 60 * 2; % this is a tray stack height at 24 inch spacing... so basically tower height
F_s_dist1 = 1; % spacing of trays in feet parameter
F_t_dist1 = 0; % type of tray used for the tower, seive in our case
F_m_dist1 = 1.7; % material choice for the tower
F_c_dist1 = F_s_dist1 + F_t_dist1 + F_m_dist1;
Dist_1_trays = (MnS/280) * 4.7 * D_dist1^1.55 * H_dist1 * F_c_dist1;

F_p_dist1_tower = 1.2; % under 300 psi
F_m_dist1_tower = 2.25; %clad stainless

F_c_dist1_tower = F_m_dist1_tower * F_p_dist1_tower;
Dist_1_pves = (MnS/280) * (101.9 * D_dist1^1.066 * H_dist1^0.82 * F_c_dist1_tower);

A_dist1_hexr = 10.7639 * 1.2e7/ (Tlm * 820) ; %given in ft^2
A_dist1_hexc = 10.7639 * 1.2e7/ (Tlm * 770) ; %given in ft^2

F_d_dist1_hexr = 1.35; % design must be kettle
F_p_dist1_hexr = 0.1; % for 1600 kpa that is under 300psi
F_m_dist1_hexr = 3.75;
Fc_dist1_hexr = (F_d_dist1_hexr + F_p_dist1_hexr) * F_m_dist1_hexr;

F_d_dist1_hexc = 0.85; % just normal condensor
F_p_dist1_hexc = 0.1;
F_m_dist1_hexc = 3.75;
Fc_dist1_hexc = (F_d_dist1_hexc + F_p_dist1_hexc) * F_m_dist1_hexc;

Dist_1_hex = ((MnS/280)* 101.3 * A_dist1_hexr ^ 0.65 * (2.29 + Fc_dist1_hexr)) + ((MnS/280)* 101.3 * A_dist1_hexc ^ 0.65 * (2.29 + Fc_dist1_hexc));

Dist_1_CAPEX = Dist_1_trays + Dist_1_pves + Dist_1_hex;

D_dist2 = 1.5 * 3.281;
H_dist2 = 14 * 2;
F_s_dist2 = 1; % spacing of trays in feet
F_t_dist2 = 0; % type of tray used for the tower, seive in our case (CAN BE CHANGED)
F_m_dist2 = 1.7; % material choice for the tower
F_c_dist2 = F_s_dist2 + F_t_dist2 + F_m_dist2;
Dist_2_trays = (MnS/280) * 4.7 * D_dist2^1.55 * H_dist2 * F_c_dist2;

F_p_dist2_tower = 1.2; % under 300 psi
F_m_dist2_tower = 2.25; %clad stainless
F_c_dist2_tower = F_m_dist2_tower * F_p_dist2_tower;
Dist_2_pves = (MnS/280) * (101.9 * D_dist2^1.066 * H_dist2^0.82 * F_c_dist2_tower);

A_dist2_hexr = 10.7639 * 3086e3/ (Tlm * 820) ; %given in ft^2
A_dist2_hexc = 10.7639 * 2760e3/ (Tlm * 770) ; %given in ft^2

F_d_dist2_hexr = 1.35; % this is a kettle reboiler
F_p_dist2_hexr = 0.1;

```
F_m_dist2_hexr = 3.75;
Fc_dist2_hexr = (F_d_dist2_hexr + F_p_dist2_hexr) * F_m_dist2_hexr;


F_d_dist2_hexc = 0.85;
F_p_dist2_hexc = 0.1;
F_m_dist2_hexc = 3.75;
Fc_dist2_hexc = (F_d_dist2_hexc + F_p_dist2_hexc) * F_m_dist2_hexc;

Dist_2_hex = ((MnS/280)* 101.3 * A_dist2_hexr ^ 0.65 * (2.29 + Fc_dist2_hexr)) +
((MnS/280)* 101.3 * A_dist2_hexc ^ 0.65 * (2.29 + Fc_dist2_hexc));

Dist_2_CAPEX = Dist_2_trays + Dist_2_pves + Dist_2_hex;



Dist_capex = Dist_1_CAPEX + Dist_2_CAPEX;


%% PSA costing (for both water and hydrogen)
W_min_psa_water = (2272/3.6) * Tsep_water * R * (.1683*log(.1683/.1676) +
.3767*log(.3767/.3751) + .4156*log(.4156/.4138) + ...
    0*log(xD1/z(4)) + 0*log(xE1/z(5)) + 0.0395*log(0.0395/0.0393))...
    + FS_postflash * Tsep_water * R * xS2 * log(xS2/0.0042);
psa_capex_water = c * lambda * W_min_psa_water; % might need to be tweaked to get
exact cost of PSA system with an adsorbant as well

% W_min_psa_H2 = 849.8 * (1000/3600) * Tsep_H2 * R * (log(1/0.9915)) + ...
    %102.5 * Tsep_H2 * R * (0.0718*log(0.0718/0.0077) + 0.0068*log(0.0068/0.0007) +
0.9212*log(0.9212/0.9915));
D_psa_H2 = 0.12 * 3.28;
H_psa_H2 = .46 * 3.28;
F_m_psa_H2 = 2.25;
F_p_psa_H2 = 1.2;
F_c_psa_H2 = F_m_psa_H2 * F_p_psa_H2;
psa_capex_H2 = (MnS/280)*(101.9 * D_psa_H2^1.066 * H_psa_H2 * (3.18 +
F_c_psa_H2));

PSA_CAPEX = psa_capex_water + psa_capex_H2;


%% Net Present Value calc


years = (0:18)';
```

entpz = 0.15;
tax = 0.27;
dscn = (1 + entpz) .^ years;
% ISBL_nopsa = PFR_cost + furnace_cost + sep_capex+furnace_cost2; %not including heat exchanger at this scope
% OSBL_nopsa = 0.4 * ISBL_nopsa;   %more in depth would be to find amount of electricity used from outsource
% contingency_nopsa = (ISBL_nopsa + OSBL_nopsa) * 0.25;

ISBL_psa = PFR_cost + heat_ex_CAPEX + cool_ex_CAPEX + Dist_capex + flash_CAPEX + furnace_tot_cost + PSA_CAPEX;
% furnace_cost + psa_capex + furnace_cost2;

OSBL_psa = 0.4 * ISBL_psa;   %more in depth would be to find amount of electricity used from outsource
contingency_psa = (ISBL_psa + OSBL_psa) * 0.25;
% TFCC_nopsa = 1.3* (ISBL_nopsa + OSBL_nopsa + contingency_nopsa); %1.3 for indirect cost
TFCC_psa = 1.3* (ISBL_psa + OSBL_psa + contingency_psa);
salvage = 0.05;

%CO2_prod_cost = 125 * (3 * FD(i) + FE(i) + 4 * FF(i)) * 44.01 * 3600 * 24 * 7 * 50 /(1e+6); % [$/annum]
% CO2_prod_cost_nopsa = 125/1e9*3600*24*7*50/802*44.01*(Q_furn+Q_furn_streamHeating+lambda*W_min_sep);

CO2_prod_cost_psa = 125/1e9*3600*24*7*50/802*44.01*(Q_furn+Q_furn_streamHeating+lambda*W_min_psa_water); %[$/annum]

ETH_stock_cost = 1060/3.6 * 200 * 30.07 * 3600 * 24 * 7 * 50 /(1e+6); % cost of fresh ethane feed in [$/annum]
Steam_cost = 2.38 * 805/3.6 *18.02 * 3600 * 24 * 7 * 50 /(1e+6); % 2 bar and 121C steam inlet to reactor in [$/annum]
% NG_cost_nopsa = 3 * (1e-9) * (3600*24*7*50) * (Q_furn+Q_furn_streamHeating + lambda*W_min_sep) ;

NG_cost_psa = 3 * (1e-9) * (3600*24*7*50) * (Q_furn+Q_furn_streamHeating + lambda*W_min_psa_water) ; % $/mol * mol/annum .... get mol from converison down volume of rxtr
% MAKE SURE THIS IS IN $/YEAR NOT $MM/YEAR
Refrige_cost_psa = sum((30240000/1)*(Q_coolers_streams./1e9).*exp(2.4647 - 0.01812 .*Q_coolers_Temps)); % multiply each duty by its respective neccesary refridgerant cost.... $/kg * kg/kJ * power/time -> MM$/annum

WC = 2/12 * (ETH_stock_cost+Steam_cost); % 2 months of raw materials

% capex_nopsa = [1/4*TFCC_nopsa ; 1/4 * TFCC_nopsa; 1/4 * TFCC_nopsa ;1/4*TFCC_nopsa + WC;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

capex_psa= [1/4*TFCC_psa ; 1/4 * TFCC_psa; 1/4 * TFCC_psa ;1/4*TFCC_psa + WC;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];

% rev_none = (900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6)) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i)));   % mol/s * KJ/mol * 3$/GJ * 1GJ/1e+6KJ   % WITHOUT PSA
% rev_psa = ((FB(i) * 28.06 * 900 + 0.9* FC(i) * 2.02 * 1400) * 3600 * 24 * 7 * 50 /(1e+6)) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (2220 * FD(i) + 802 * FE(i) + 2878 * FF(i)+ 286 * FC(i)*0.1));
% rev_none = 900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6);
rev_psa = 900* FB(i) * 28.06 * 3600 * 24 * 7 * 50 /(1e+6);

% byprodrev_none = (3 * 3600 * 24 * 7 * 50 /(1e+6) * (286 * FC(i) + 2220 * FD(i) + 890 * FE(i) + 2878 * FF(i)));
% byprodrev_psa = 0.9 * FC(i) * 2.02 * 1400 * 3600 * 24 * 7 * 50 /(1e+6) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (2220 * FD(i) + 802 * FE(i) + 2878 * FF(i)+ 286 * 0.1 * FC(i))); % ALL hydrogen can be sold off due to flash exploit
byprodrev_psa = 864.2/3.6 * 2.02 * 1400 * 3600 * 24 * 7 * 50 /(1e+6) + (3 * 3600 * 24 * 7 * 50 /(1e+6) * (0* 2220 * FD(i) + 0* 802 * FE(i) + 2878 * 92.45/3.6 + 286 * 96/3.6 + 22.4/3.6* 1420)); % ALL hydrogen can be sold off due to flash exploit

revenue_psa = rev_psa * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1];

REV = revenue_psa; % matrix of revenue for no psa and with psa respectively
AGS = 0.05 * REV; %gives just a vector for the payment to workers / administration

VCOP_psa = (CO2_prod_cost_psa + ETH_stock_cost + Steam_cost + NG_cost_psa + Refrige_cost_psa - byprodrev_psa - expander_OPEX + compressor_OPEX); %variable costs of production with psa... essentially a OPEX
FCOP_psa = AGS(end); % fixed costs of production with psa

COM_psa = (VCOP_psa + FCOP_psa) * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1;1;1;1]; % energy costs and continuous raw material costs

GRprof_psa = REV - COM_psa;

cost_basis_psa = 11/10 * (2.28 * ISBL_psa);

```matlab
    depriciation_psa = cost_basis_psa *
[0;0;0;0;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0;0;0;0;0]; %ten year linear dpereiciation model


    tax_inc_psa = GRprof_psa - depriciation_psa;


    tax_paid_psa = tax * tax_inc_psa;

    CashFlow_psa = (REV(:) - COM_psa - depriciation_psa) .* (1 - tax) - capex_psa +
depriciation_psa;

    CashFlow_psa(19,1) = CashFlow_psa(19,1) - TFCC_psa*salvage;

    PV_psa = CashFlow_psa./dscn;

    NPV_psa = zeros(19,1);


    for j = 2:length(years)

       NPV_psa(1) = PV_psa(1);
       NPV_psa(j) = PV_psa(j) + NPV_psa(j-1);
    end

    NV = zeros(19,1);

    for j = 1:length(years)

       NV_psa(j) = sum(CashFlow_psa,1:j);
    end



    % CFD_PSA = table(years, capex, REV(:,n), COM, GRprof, depriciation, tax_inc,
tax_paid, CashFLow, PV, NPV, NV, ...
        % 'VariableNames', ['Years', 'Rev', 'COM', 'GRprof', 'Dep', 'Taxable Inc', 'Taxes Paid',
'Cash Flow', 'PV', 'NPV', 'NV']);
    CFD_PSA = table(years, capex_psa, REV(:), COM_psa, GRprof_psa, depriciation_psa,
tax_inc_psa, tax_paid_psa, CashFlow_psa, PV_psa, NPV_psa, NV_psa');
    Money_PSA(i) = CFD_PSA{19,"NPV_psa"};



end
```

```matlab
% figure(1)
% plot(XA,Money_PSA/1e6,'g','LineWidth',2)
% ylim([0 5e2])
% xlabel('Single pass conversion')
% ylabel('Net Present Value $MM/annum')
% figure(2)
% plot(Vplant/1e3,Money_PSA/1e6,'k','LineWidth',2)
% ylim([0 5e2])
% xlabel('Reactor Volume [m^3]')
% ylabel('Net Present Value $MM/annum')
[x,y_psa] = max(Money_PSA);
sprintf('Max NPV PSA $MM/annum:  %0.5g',x/1e6)
sprintf('Reactor Volume m^3 : %0.5g',Vplant(y_psa)/1e3)
% [x,y] = max(Money_No);
% sprintf('Max NPV No PSA $MM/annum:  %0.5g',x/1e6)
% sprintf('Reactor Volume m^3 : %0.5g',Vplant(y)/1e3)


% sep_capex_per = sep_capex/ISBL_nopsa;
% pfr_nopsa_per = (PFR_cost)/ISBL_nopsa;
% furn_nopsa_per = furnace_cost/ISBL_nopsa;
figure(1)
% X = [pfr_nopsa_per,sep_capex_per,furn_nopsa_per,furnace_cost_tot/ISBL_nopsa];
% Labels = {'PFR','Separations',' Pyrolysis Furnace','Stream Heating Furnace'};
% xPercent = X / sum(X) * 100;
% newLabels = [];
% for i=1:length(X)
%    newLabels = [newLabels {sprintf('%s (%.1f%%)', Labels{i}, xPercent(i))}];
% end
% pie(X, newLabels);
% title('ISBL Operating Expenses No PSA')

psa_capex_per = psa_capex/ISBL_psa;
pfr_psa_per = (PFR_cost)/ISBL_psa;
furn_psa_per = furnace_cost/ISBL_psa;

figure(2)
X = [pfr_psa_per,psa_capex_per,furn_psa_per,furnace_cost_tot/ISBL_psa];
Labels = {'PFR','Separations',' Pyrolysis Furnace','Stream Heating Furnace'};
xPercent = X / sum(X) * 100;
newLabels = [];
for i=1:length(X)
   newLabels = [newLabels {sprintf('%s (%.1f%%)', Labels{i}, xPercent(i))}];
end
pie(X, newLabels);
```

title('ISBL Operating Expenses No PSA')

figure(3)
X = [ETH_stock_cost,CO2_prod_cost_psa,NG_cost_psa+Steam_cost,AGS(end)];
Labels = {'Fresh Ethane','CO2 Tax','Utilities','AGS'};
xPercent = X / sum(X) * 100;
newLabels = [];
for i=1:length(X)
    newLabels = [newLabels {sprintf('%s (%.1f%%)', Labels{i}, xPercent(i))}];
end
pie(X, newLabels);

%%% Sensitivity Analysis

% Energy_per_kg =
(3600*7*24*50)*(Q_furn_streamHeating+Q_furn_rxn+35*W_min_psa)/((200*10^6))/1e6;
% Energy_per_PJ =
(3600*7*24*50)*(Q_furn_streamHeating+Q_furn_rxn+35*W_min_psa)/1e15;
% CO2kg_per_kg =
((3600*7*24*50)*(Q_furn_streamHeating+Q_furn_rxn+35*W_min_psa)/802/1e6*44.01)/(200*1e6)
% NGkg_per_kg=
(3600*7*24*50)*(Q_furn_streamHeating+Q_furn_rxn+35*W_min_psa)/802/1e6*16/(200*1e6)
% Q_furn_streamHeating/1e6

PFR code to get Initial Conversion/Selectivity

clc; clear; close all;
%%% Optimize for NPV

T = 825+273;
Ptot = 200;
R = 8.314;
MR = 0.6;

%%% Species Flows
FA0 = 1; %Used for XA and S only, needs to be scaled
Vmax = 50000;
[V,F] = getFETi(FA0,Vmax,T,Ptot);

```matlab
FA = F(:, 1);
FB = F(:, 2);
FC = F(:, 3);
FD = F(:, 4);
FE = F(:, 5);
FF = F(:, 6);
FS = F(:, 7);
figure(1)
plot(V, FA, 'b', V, FB, 'g', V, FC, 'r', V, FD, 'c--', V, FF, V, FS, 'k', "LineWidth", 2);
legend('Ethane', 'Ethylene', 'Hydrogen', 'Propane/Methane', 'Butane','Steam',
"Location","best");
xlabel('Reactor Volume [L]','FontWeight','bold');
ylabel('Species Flows [mol/s]','FontWeight','bold');


box OFF
xlim([0 100])
%title('Species Flows at T =',T(i))
%% Conversion + Selectivity Calculations
XA = (FA0 - FA)/FA0;
S2 = FB ./(FA0.*XA); %for ethylene
S2 = (FB - 0)./(FA0 -FA);
S3 = FC ./((FA0).*XA); %for hydrogen
S4 = FD ./((FA0).*XA); %for propane
S5 = S4; %for methane
S6 = FF ./((FA0).*XA); %for butane
%flow rate and tau
Ftot = FA + FB + FC + FD+ FE +FF + FS;
q0 = R*T/Ptot*(1+MR);
tau = V./q0;
tau = V*Ptot./(R*T*(1+MR));
%Product flows scaled to plant volume
%mol/s basis
FBplant = 235.7*ones(length(S2),1);

% for i = 1:length(S2)
%     LHS = [-2 0 -1; 0 0 1; 1 -1 0];
%     RHS = [FBplant(i)./S2(i)*(S3(i)-1); FBplant(i)*(S3(i)/S2(i)-1);0];
%     s = LHS\RHS;
%
```

```
% FEplant(i) = s(1);
% FDplant(i) = s(2);
% FFplant(i) = s(3);
% FFAplant(i) = FBplant(i)./S2(i);
% FCplant(i) = FBplant(i).*S3(i)./S2(i);
% FSplant(i) = FFAplant(i)*MR;
% RAplant(i) = FBplant(i)./(S2(i)).*(1-XA(i))./XA(i);
RAplant = FBplant./(S2).*(1-XA)./XA;
FAplant = RAplant;
FFAplant = FBplant./S2;

FCplant = FBplant.*S3./S2;
FDplant = FBplant./2.*(1-2.*S3+S2)./S2;
FEplant = FDplant;
FFplant = FBplant.*(S3-S2)./S2;
FSplant = MR*(RAplant+FFAplant);

FFSplant = (RAplant+FFAplant)*MR;
FlowToSeparations = RAplant+FBplant+FCplant+FDplant+FEplant+FFplant+FSplant;

v =R*T*FBplant*(1+MR)./(Ptot.*S2.*XA); %volumetric flow rate
Vplant = tau.*v;

%plant volume required to
%Vplant = V.*(RAplant+FFAplant+FFSplant)./(FA + FB + FC + FD + FE + FF + FS);


%% MATLAB DELIVERABLES
%% 1 Selectivity vs. Conversion
figure(2)
plot(XA, S2,"LineWidth",2)
xlabel('Conversion of Ethane')
ylabel('Selecivity of Ethylene')

%%  2 Volume vs. Conversion
figure(3)
plot(XA, Vplant,'b',"LineWidth",2)
xlabel('Conversion of Ethane','FontWeight','bold')
ylabel('Reactor Volume [L]','FontWeight','bold')
ylim([0 50000])
```

```
box OFF

%% 3 Fresh Feed Ethane vs. Conversion
figure(4)
%outlet flow vs volume of reactor
loglog(Vplant, FAplant, 'b', Vplant, FBplant, 'g',...
    Vplant, FCplant, 'r', Vplant, FDplant, 'c--',...
     Vplant, FFplant, Vplant, FSplant, 'k', "LineWidth", 2);
legend('Ethane', 'Ethylene', 'Hydrogen', 'Propane/Methane', 'Butane','Steam'
,"Location","best");
xlabel('Reactor Volume [L]','FontWeight','bold');
ylabel('Species Flows [mol/s]','FontWeight','bold');
box OFF
% plot(XA, FFAplant, "LineWidth", 2);
% xlabel('Conversion of Ethane');
% ylabel('Feed Ethane [kgmol/hr]');
% ylim([0 5000]);
% xlim([0 1]);
%% 4 Product Flows vs. Conversion
figure(5)
plot(XA, RAplant./3.6, 'b', XA, FBplant./3.6, 'g',...
    XA, FCplant./3.6, 'r', XA, FDplant./3.6, 'm-.',...
    XA, FEplant./3.6, 'c--', XA, FFplant./3.6, 'k',XA, FSplant./3.6, "LineWidth", 2);
legend('Ethane', 'Ethylene', 'Hydrogen', 'Propane', 'Methane', 'Butane','Steam',
"Location","best");
title('Outlet Flows [kgmol/hr] vs. Conversion')
xlabel('Conversion');
ylabel('Species Flows [kgmol/hr]');
ylim([0 500])

%% 6 Feed Ethane vs. Conversion vs. Selectivity
figure(6)
subplot(2,1,2)
hold on
plot(XA,FAplant, "LineWidth", 2)
title('Feed Flow Ethane [kgmol/hr] vs. Conversion')
xlabel('Conversion');
ylabel('Feed Ethane [kgmol/hr]');
ylim([0 10000]);
xlim([0 1]);
```

```
subplot(2,1,1)
plot(S2,FAplant, "LineWidth", 2)
title('Feed Flow Ethane [mol/s] vs. Selectivity')
xlabel('Selectivity of Ethylene');
ylabel('Feed Ethane [kgmol/hr]');
ylim([0 10000]);
xlim([0 1]);
%%% 5 Recycle Flow rate vs. Conversion
figure(7)
plot(XA, RAplant,"LineWidth",2)
xlabel('Conversion of Ethane')
ylabel('Recycle Flow Rate [mol/s]')
title('Reycle Flow Rate [mol/s] vs. Conversion')
ylim([0 5000])
%%% 7 Flow Rate to separation system
figure(8)
plot(XA, FlowToSeparations,"LineWidth",2)
xlabel('Conversion')
ylabel('Separations Flow Rate [mol/s]')
title('Separations Flow Rate [mol/s] vs. Conversion')
ylim([0 5000])

%%% 8 Mol Fraction to separation system
figure(9)
plot(XA, RAplant./FlowToSeparations, XA, FBplant./FlowToSeparations,...
    XA, FCplant./FlowToSeparations,XA, FDplant./FlowToSeparations, ...
    XA, FEplant./FlowToSeparations,XA, FFplant./FlowToSeparations,XA,
FSplant./FlowToSeparations,...
    "LineWidth",2)
legend('Ethane', 'Ethylene', 'Hydrogen', 'Propane', 'Methane', 'Butane','Steam',
"Location","best");
xlabel('Conversion')
ylabel('Separations mol fraction')
title('Separations mol fraction vs. Conversion')
```

Sensitivity Code

```
clc;clear;
```

```matlab
Variables = {'Cost Basis[$MM]','Contingency[$MM]','OSBL [$MM]','Indirect
Cost[$MM]','CO_2 cost[$/MT]','H_2 value[$/MT]','Fuel
cost[$/GJ]','ISBL[$MM]','Construction time[yrs]',...
    'Interest[%]','Raw mat cost[$/MT]','TFCC[$MM]','Refrigeration cost[$/GJ]','Ethylene
production[kta]','Ethylene Value[$/MT]'};

LB_affect =
[28.4,28.4,139.3,140.3,157.4,132.1,139.5,133.2,112.9,131.8,127.3,200.6,122.4,128.3,126.9];

UB_affect =
[220.4,220.4,50.1,104,97.6,109,79.1,115.6,135.9,105.8,116.9,48.2,129.5,114.6,117.9];


Nominal_NPV = 124.4 ;

total = abs(-LB_affect + UB_affect);
[total,ind] = sort(total,'ascend');
LB_affect = LB_affect(ind);
UB_affect = UB_affect(ind);


figure()
a = barh(LB_affect,'FaceColor', [0.8500 0.3250 0.0980]); % Dark orange
hold on
b = barh(UB_affect,'FaceColor', [0.3010 0.7450 0.9330]); % Light blue
legend([a, b], {'Variable loss', 'Variable gain'}, 'Location', 'Southwest');
c = get(a,'BaseLine');
set(c,'BaseValue',Nominal_NPV);
set(gca,'yticklabel',Variables)
xtickformat('$%,.0f MM')
```
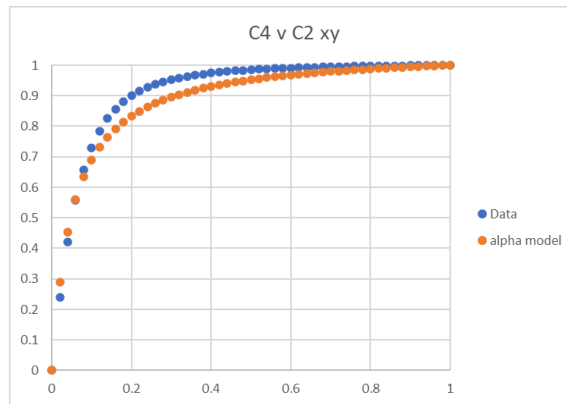
J - Underwood excel sheet

Figure J.1: Underwood graph for ethane to butane giving an α=20
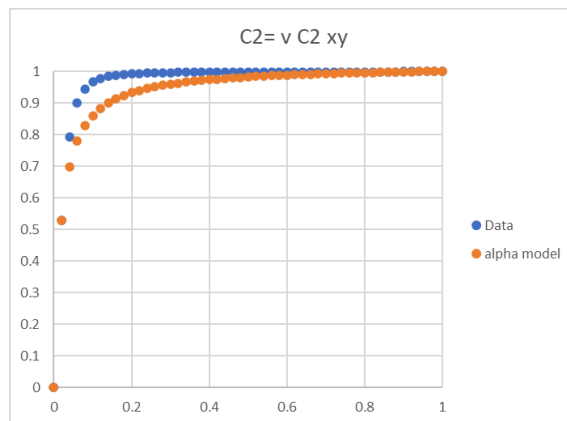

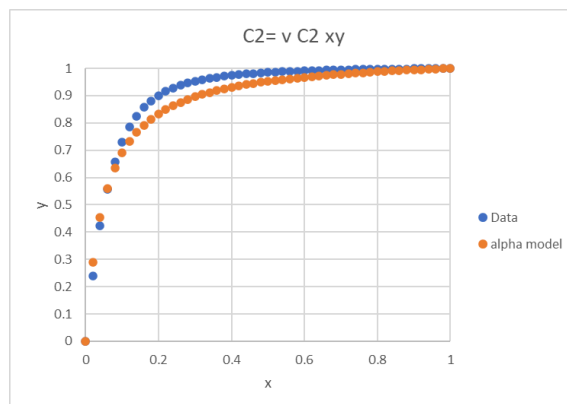Figure J.2: Underwood graph for ethylene to butane giving an α=50

Figure J.4: Underwood graph for ethylene to butane giving an α=20