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**Capstone Project II**

**Report IV**

Design of Plant for Industrial Production of Ethylene in Kazakhstan  
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## **List of Abbreviations**

ACT – Acetylene  
BACT – Best Available Control Technology  
BDN – 1,3-Butadiene  
CAPEX – Capital Expenditure  
CIS – Commonwealth of Independent States  
CSTR – Continuous Stirred Tank Reactor  
EBIT – Earnings Before Interest and Taxes  
ESI – Electronic Supplementary Information  
ETH – Ethane  
ETLN – Ethylene  
F – Molar Flow Rate  
GDP – Gross Domestic Product  
GHG – Greenhouse Gases  
GOST – Government standard  
HRG – Hydrogen  
HX – Heat Exchanger  
ISBL – Inside Battery Limits  
LDAR – Leak Detection and Repair  
LMTD – Log Mean Temperature Difference  
MACT – Maximum Achievable Control Technology  
MET – Methane  
MTO – Methanol-To-Olefins  
OCM – Oxidative Coupling of Methane  
OPEX – Operating Expenditure  
OSBL – Outside Battery Limits  
P – Pressure  
PE – Polyethylene  
P&ID – Piping and Instrumentation Diagram  
PFD – Process Flow Diagram  
PFR – Plug Flow Reactor  
PM – Particulate Matter  
PRLN – Propylene  
PRO – Propane  
T – Temperature  
U – Overall Heat Transfer Coefficient  
V – Volume  
VOC – Volatile Organic Compound

## Chapter 1. Process Introduction

### 1.1 Ethylene Properties

Ethylene (IUPAC name: ethene, CAS No. 74-85-1) is the simplest olefin, consisting of two carbon atoms connected by a double bond ( $C_2H_4$ ). It is a colorless, flammable gas with a faint sweet odor and is non-corrosive under standard conditions. Ethylene is highly reactive due to its double bond, making it one of the most important building blocks in the petrochemical industry [1]. The table below displays the general properties of ethylene:

**Table 1.** Physical and chemical properties of ethylene [1, 2]

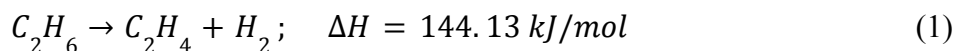
| Chemical structure | Properties        |                          |
|--------------------|-------------------|--------------------------|
| $H_2C=CH_2$        | IUPAC Name        | Ethene                   |
|                    | Molecular Formula | $C_2H_4$ , $H_2C = CH_2$ |
|                    | Appearance        | Colorless gas            |
|                    | Molecular weight  | 28.0532 kg/kmol          |
|                    | Melting Point     | -169.18 °C               |
|                    | Boiling Point     | -103.8 °C                |
|                    | Density           | 1.1938 kg/m <sup>3</sup> |

### 1.2 Review of the Production Routes

#### 1.2.1 Steam Cracking of Natural Gas

Steam cracking of natural gas (ethane) is a non-catalytic thermal process that converts light paraffins into ethylene as a result of free radical chain reactions. Although the process is energy-intensive, it achieves a comparatively high ethylene yield.

The principal cracking step for ethane is endothermic dehydrogenation [1]:

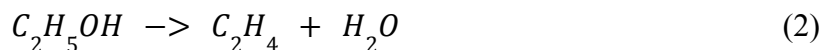


Steam cracking runs at COT 850-950 °C. The effluent is quenched in the TLE to 650°C to limit secondary reactions [2]. Downstream, the dry gas is compressed to 30 bar, pre-cooled to -140 °C, and light gases are removed. Then the  $C_2$  is split near -25 °C and 34 bar to yield approximately 99.9 mol% ethylene, with ethane recycled [3].

### 1.2.2 Ethanol Dehydration

An alternative pathway to produce ethylene is the catalytic dehydration of ethanol. The process is achieved in two major stages, namely main ethanol dehydration reaction and consequent purification of ethylene products [4].

The dehydration of ethanol to ethylene occurs through a simple endothermic reaction:

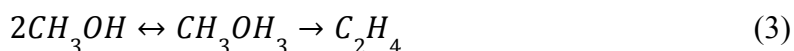


During the reaction, an acid catalyst first protonates the hydroxyl group, which then leaves as a water molecule. The conjugate base of the catalyst then proceeds to deprotonate the methyl group, so that the hydrocarbon rearranges into an ethylene molecule. Tsao et al. have developed this process in a fluidized bed reactor using silica-alumina-oxide catalyst, achieving a one-way conversion rate of 99.5% and ethylene yield greater than 99% [4].

The process typically operates at temperatures of 300–500 °C, depending on the catalyst used, and at pressures ranging from 0.1 to 0.2 MPa. Under optimized conditions, ethanol conversion above 95% and ethylene selectivity exceeding 98% can be achieved. The reaction is usually carried out in either a fixed-bed tubular reactor packed with solid acid catalysts, or the fluidized-bed and membrane reactors [4].

### 1.2.3 Methanol-to-Olefins Method

Unlike conventional steam cracking, MTO provides an alternative route to basic petrochemical building blocks from non-oil resources, including coal and natural gas. This makes it an attractive option for regions seeking to diversify feedstock sources away from crude oil [5].



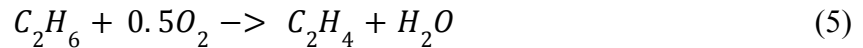
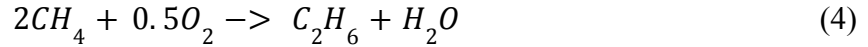
The MTO process involves a series of catalytic reactions that convert methanol into light olefins. The initial step is methanol dehydration, which produces dimethyl ether (DME) and water. Although DME is a stable intermediate, it undergoes further reactions on the sites of zeolite catalysts. These reactions yield light olefins in the C<sub>2</sub>-C<sub>5</sub> range, particularly ethylene and propylene [6].

These processes operate at high temperatures (400-500°C) and medium pressures (0.1-0.3 MPa), achieving nearly complete methanol conversion while maintaining moderate selectivity toward ethylene and propylene [5]. Despite these technological advancements, the overall process is highly exothermic and requires careful heat management, as well as extensive downstream separation systems to isolate polymer-grade products [7].

#### *1.2.4 Oxidative Coupling of Methane*

Oxidative Coupling of Methane (OCM) is considered a laboratory-scale process of converting methane into ethane under the application of oxygen and heterogeneous catalysts [8]. Ethane is then converted to the desired product - ethylene, by a dehydrogenation process with catalytic or thermal gas-phase oxidation.

The main reactions that are present in the OCM method are the following [9]:



The process consists of many side reactions. Therefore, the yield of the reaction often is reduced. Eq. (4) represents the formation of ethane, and Eq. (5) demonstrates the heterogeneous catalytic oxidative dehydrogenation of ethane to ethylene and water.

The feed is inserted at 25°C with a pressure of 3 bar and heated to an operating temperature of 810°C before entering the reactor. On the second stage, the mixture is cooled to 40°C before entering the water separation section. The overhead is fed to the absorber at 12 bar, where the carbon dioxide is removed at a temperature of 150°C. Finally, the ethylene and ethane are separated in a distillation column with the compressed and cooled stream at 30 bar and -25°C [9].

#### ***1.3 Process Selection***

Table 2 summarizes the principal industrial methods of ethylene, lists feedstocks, key products, catalysts, and typical operating conditions, to highlight their comparative advantages and limitations.

**Table 2.** Comparison of different ethylene production methods

| Method name<br>Property                        | Steam cracking                                                          | Ethanol<br>dehydration                                                                                        | Methanol-to-Olefins                      | Oxidative coupling<br>of methane |
|------------------------------------------------|-------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------|------------------------------------------|----------------------------------|
| Feedstock                                      | Gas (75 vol%) and steam (25 vol%)                                       | Ethanol                                                                                                       | Methanol (from coal or natural gas) [10] | Methane and oxygen               |
| Main products                                  | 37.7 mol% ethylene, 40.7 mol% hydrogen, 3.3 mol% methane, and 15.1 mol% | Ethylene (polymer-grade) + water; minor DEE, traces of heavies                                                | Light olefins (ethylene, propylene) [11] | Ethylene                         |
| Catalysts                                      | None                                                                    | $\gamma$ -Al <sub>2</sub> O <sub>3</sub> , silica-alumina, heteropolyacids, zeolites (HZSM-5, HBeta, SAPO-34) | SAPO-34 [12]                             | Li/MgO                           |
| Temperature, °C                                | 800–950                                                                 | 300–500                                                                                                       | 400–500                                  | 810                              |
| Yield of ethylene                              | Yield of 37.7% [13]                                                     | Yield > 99%                                                                                                   | Industrial-grade yield 16.721% [12]      | Yield 25% [14]                   |
| Production cost (per ton of ethylene produced) | Low, \$832 (€710) [13]                                                  | High, €4000 [18]                                                                                              | High, €3260 [18]                         | Medium, €931.96 [18]             |

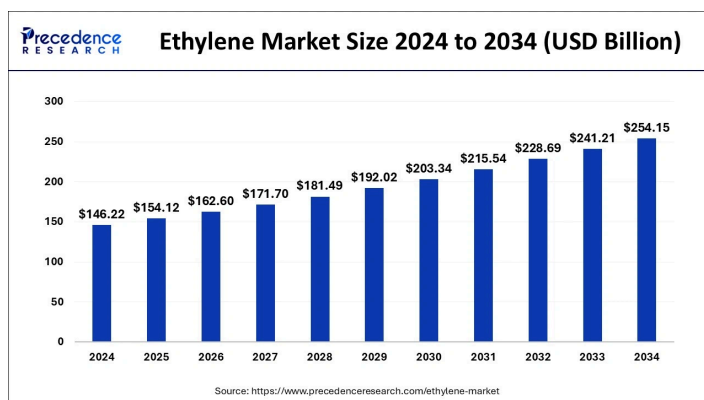
Although all processes have high energy consumption as presented in Table 2, oxidative coupling has not been implemented as an industrial method, so cannot be chosen as a suitable pathway. Considering feedstock, the most available method in Kazakhstan is steam cracking because of rich reserves of oil and gas, while ethanol and methanol are not readily available for purchase, due to the absence of domestic production facilities [19]. Additionally, steam cracking proved to be most advanced presently with 37.7% molar yield [20], while methanol-to-olefins yields 16.7% [21]. Even though ethanol dehydration has much higher yields of greater than 99% at high conversions, its production rates are significantly lower than other processes, which increases production cost up to 4000€ per ton of ethylene produced [22], which is more than steam cracking and methanol-to-olefins, at 709€ per ton and 3260€ per ton of ethylene produced respectively.

Overall, the factors in Table 2 mention the advantages and disadvantages of the manufacturing methods based on production cost, yield, environmental impact, operating conditions, usage of catalysts, feedstock needed and main products of the options. According to the listed characteristics, compared to other ethylene manufacturing methods, steam cracking represents the most efficient way of ethene production.

## 1.4 Market Analysis

### 1.4.1 Global Market Analysis of Ethylene Production

In the petrochemical industry, the ethylene production market is considered one of the largest and most demanding economical segments. In 2024, the world ethylene market was evaluated at USD 146.22 billion, expected to grow to USD 254.25 billion in 2034. In 2025, the production market was estimated at USD 154.12 billion, whereas the compound annual growth rate (CAGR) is evaluated as 5.68 per cent, as can be observed in Figure 1 [23].



**Figure 1.** Ethylene market size in 2024-2034 [23]

The projected growth of the ethylene market can be attributed to the rising demand for polyethene products, such as linear low-density and high-density polyethene. In 2024, about 57 per cent of ethylene application was accounted for by the polyethene segment, while approximately 52 per cent of revenue was contributed by the end-use packaging industry [23]. Additionally, the growing market of ethylene is attributed to the demand for ethylene-propylene diene monomer (EPDM), used for light-weight vehicles manufacturing [24].

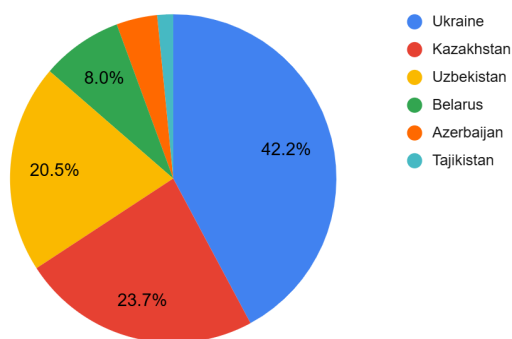
### 1.4.2 Ethylene Market Analysis in CIS Regions

Due to the unavailability of data regarding the ethylene demand in CIS regions, the demand for polyethylene (PE) was analysed and compared, as the designed ethylene-producing plant is to account for 25 percent of the demand in the CIS market. Overall, the global polyethylene demand trend shows that in 2020, former USSR countries contributed around 3 per

cent to the global PE demand by region. At the same time, the annual growth in demand for this region was estimated to be approximately 1.1% in the period of 2019-2020 [25].

Among the countries of the Eurasian Economic Union (EEU), in 2022, the volume of imported PE was evaluated as 52.3 million metric tons in Belarus, significantly rising to 84.1 million tons in 2023. Azerbaijan's PE production and import was approximated as 24.6 million tons in 2022, increasing almost three times to 76.3 million metric tons in 2023. According to the volume of polyethylene imported from Uzbekistan, the values rose from 29.8 million metric tons in 2022 to 43.9 million tons in 2023 [26].

One of the most widely used forms of PE is polyethene terephthalate (PET), utilised as a thermoplastic polymer. The import data of PET in the CIS countries in 2019 can be observed in Figure 2.



**Figure 2.** Imports of polyethylene terephthalate (PET) in CIS countries in 2019 [27]

As it can be observed from Figure 2, the largest share of PET was imported by Ukraine. This is followed by Kazakhstan, which accounted for 23.7% of the total PET import share in the CIS region. The amount of PET imported by Uzbekistan was evaluated at 20.5 per cent of the overall imported volume, followed by Belarus, Azerbaijan, and Tajikistan.

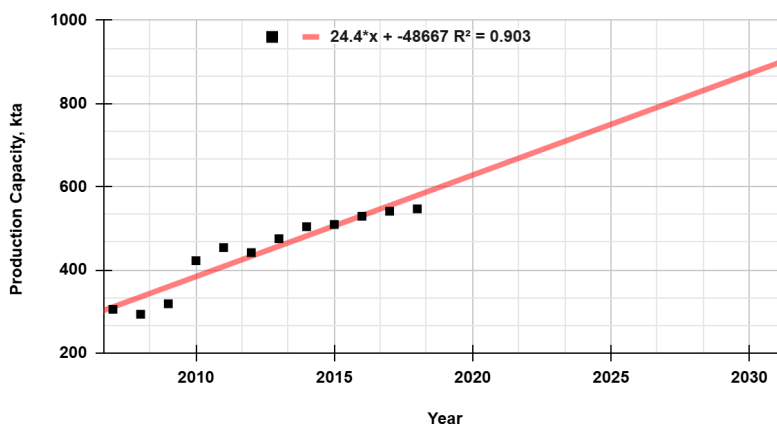
In Kazakhstan, the largest polyethene production site is to be launched in 2029. The Silleno project, developed under the shares of KazMunayGas, KMG PetroChem, Sibur, and Sinopec, is to produce 1250 kta of polyethene, whereas the cost of the project is estimated at USD 7.4 billion. Currently under design stage, this initiative is to use 1.6 million metric tons of ethane produced from 9.1 million tons of natural gas on the deposits of Tengizchevroil LLP [27].

### **1.5 Production Rate**

Due to limited data for the CIS region, ethylene production capacity was estimated using China's market data (2007-2018) as a reference. A scaling approach based on the ratio of China's and the CIS region's nominal GDPs was used to estimate CIS ethylene demand. This scaling

factor was applied to the data, and a linear regression model was then used to project demand and determine production capacity for 2030.

China's ethylene production capacity data from 2007 to 2018 [28] was used, and demand for the CIS region was derived by scaling based on nominal GDP. In 2018, China's GDP was 14.15 trillion USD [29], while the CIS (excluding Russia) was 421 billion USD [30], resulting in a scaling factor of 0.0297 (see Appendix A). Applying this factor gave an estimated CIS ethylene demand of 546.7 kta. Annual estimates were generated using the same approach, and a linear regression model was applied to forecast future demand and determine production capacity for 2030.



**Figure 3.** Predicted ethylene market in CIS

According to Figure 3, the increasing trend in CIS's ethylene production market can be modeled using the linear equation of the form  $y = 24.4 * x - 48,667$ . Based on the linear equation, the ethylene production in CIS is estimated as 743 kta in 2025. To meet the requirement of supplying ~25% of CIS demand by 2028, the projected market size for that year was used. Based on the linear model, CIS ethylene demand in 2028 is estimated at 816.2 kta, meaning the designed plant capacity is approximately 220 kta. This capacity aligns with typical ethylene production ranges of existing steam crackers, as shown by major operators in 2021 (Table 3).

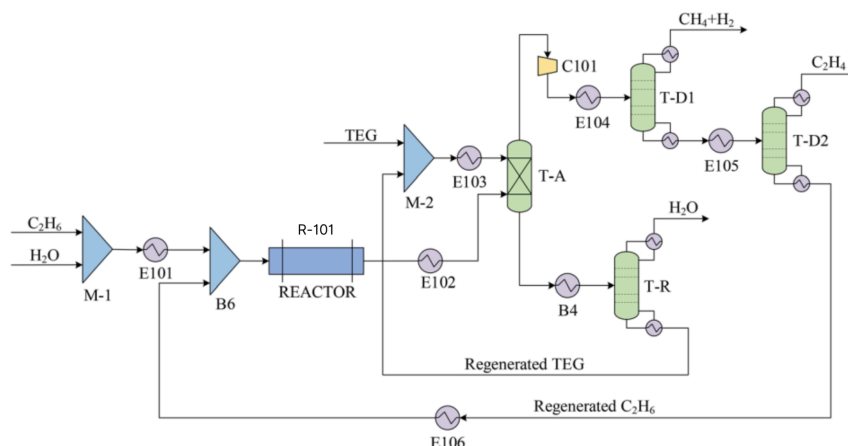
**Table 3.** Worldwide capacities of ethylene production steam cracking plants [31, 32]

| Operator       | Location              | Capacity kta |
|----------------|-----------------------|--------------|
| Sinopec        | China, Nangang        | 1,200        |
| Dow            | Germany, Boehlen      | 565          |
| LyondellBasell | France, Berre         | 470          |
| BASF           | Germany, Ludwigshafen | 220 - 400    |
| Borealis       | Finland, Porvoo       | 400          |

A polyethene plant project is currently being launched in Atyrau with a planned output capacity of 1,250 kta. According to Silleno, 1,600 kta of ethane will be supplied to a steam cracker using Lummus Technology (USA) pyrolysis [33]. Although detailed data on this technology is limited, the required ethylene capacity can be estimated: producing 1,250 kta of polyethene would require about 1,180 kta of ethylene, assuming a conversion above 95% [34].

## Chapter 2. Process Summary

### 2.1 Literature Review on Commercial PFDs

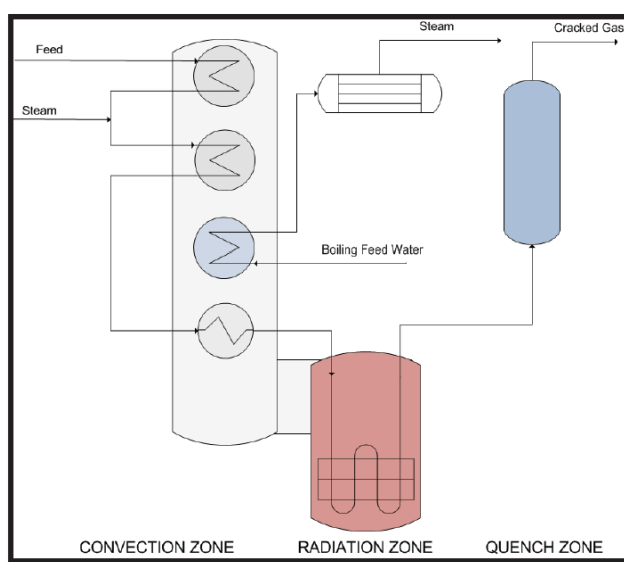
**Figure 4.** Steam cracking process flow diagram [35]

Existing literature on ethylene production via steam cracking from ethane and natural gas outlines the process flow diagram, as was demonstrated in Figure 4. Overall, the PFD of the process is divided into three distinct regions. In the first section, ethane feed enters the system alongside water in a 3:1 volume ratio, passing through the steam cracking unit. In this case, the reaction zone represents a single furnace R-101, which operates at a temperature of 950°C and a

pressure of 4.5 bars. As a result of steam cracking, ethylene is formed, accompanied by hydrogen and methane as secondary products. A small fraction of ethane remains unreacted, whereas  $C_4$  and  $C_3$  hydrocarbons undergo cracking into lighter fractions [35].

The next section on the given process flow diagram shows the water removal units T-A and T-R. In this section, water is absorbed in the T-A absorption tower, where triethylene glycol (TEG) is utilized. Water is absorbed at low temperatures, and TEG is further recovered in the T-R column to support the continuous operation of the water removal unit [35].

The final region of the observed PFD represents the ethylene treatment and recovery units C-101, T-D1, and T-D2. The dry gas is first compressed via compressor C-101 and then cooled using heat exchanger E-104. The cooled and compressed gases further proceed into the series of distillation columns. In the T-D1, methane and hydrogen are removed as overhead products, whereas heavier fractions are passed to the next distillation unit. In T-D2, ethylene is separated from the unreacted ethane and leaves the system as the overhead product, whereas ethane from the bottom products is recycled back to the first section of the system [35].



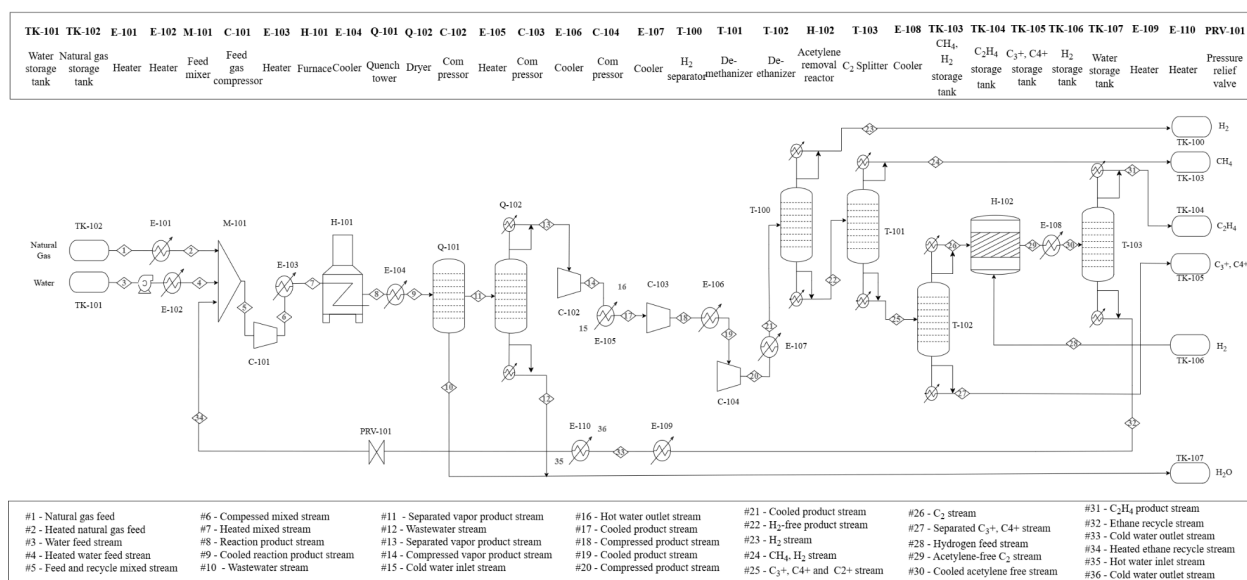
**Figure 5.** Fired furnace reactor design [36]

Most process flow diagrams showing the steam cracking of ethane to ethylene include a specific model of a furnace design. A widely used design of a steam cracking furnace includes three zones, which are the radiation, transition, and convection zones, as can be observed in Figure 5. In the first radiant zone, the endothermic cracking process occurs as a result of the heat supply from the radiant burners to the reactor coils. In the second section, the produced heat is used to provide initial preheating to the natural gas and water steam feed. The convection zone also applies a high-pressure water system in the system. The third zone of the reactor provides the quenching and cooling of the heated product stream using cold oil or water, which stops the reaction process and prevents further formation of unwanted products [36].

Therefore, furnace simulations typically model these separate regions to accurately represent heating profiles, reaction behaviour, and heat-recovery systems [36].

Despite the fact that the furnace is divided into three separate sections in the existing literature on reactor design, modeling of such a reactor unit can be difficult. Since convection and radiation zones present different regions within the reactor, distinct temperatures are required to simulate them successfully. Nevertheless, there is a limited number of sources that can provide data on the temperature differences and intermediate conditions between the reactor zones [37].

## 2.2 Proposed Design of PFD



**Figure 6. Process Flow Diagram**

Water and natural gas enter the system from the storage tanks TK-101 and TK-102, respectively. The liquid water stream is pumped to heater E-102, natural gas passes through a heat exchanger E-101, and both streams are heated to 100°C. In the mixer M-101, the feed is mixed with the recycle ethane stream #32. The stream then passes through the compressor C-101, which increases the pressure from 1 bar to 4 bar. Before entering the reaction zone in reactor H-101, the steam is heated to 850°C via E-103 heat exchanger. The H-101 reactor is a tubular plug-flow reactor operating at 4 bars and 850°C, with the design discussed further in this report.

The hot product stream leaving the reaction zone passes through the E-104 cooler. Water is removed from the reaction product stream via a quench tower Q-101 and a dryer Q-102. The wastewater stream leaves both towers in streams #10 and #12, passing to the wastewater storage

tank TK-107. The stream is then compressed from 4 bars to 10 bars by the C-101 compressor unit, which also raises the temperature of the stream by 60°C. The subsequent cooler E-105 cools the natural gas stream from 99°C to 40°C using cold water at a temperature of 25°C in the stream #15. The design of the heat exchanger E-105 is discussed further in the report. The gas stream is then compressed to 20 bars via compression units C-103 and C-104.

The stream enters the distillation column T-100, which separates hydrogen from the product stream to stream #23. Then, the stream enters the demethanizer distillation column T-101, which removes the CH<sub>4</sub> gas from the heavier C<sub>2</sub>, C<sub>3</sub>, and C<sub>4</sub> fractions in the stream #24. The hydrogen and methane flow into the storage tank TK-103, whereas the stream containing C<sub>2</sub>, C<sub>3</sub>, and C<sub>4</sub> hydrocarbons enters the de-ethanizer column T-102, which separates C<sub>2</sub> light fractions as a top stream #26, whereas the heavier C<sub>3</sub> and C<sub>4</sub> components flow into the storage tank TK-105. The design of the T-102 distillation column is discussed further in the report. The top stream from T-102 flows into the H-102 acetylene removal reactor. The hydrogen gas supplies this reaction zone from the TK-106 storage tank in stream #28, which reacts with the C<sub>2</sub>H<sub>2</sub> fraction in the stream. The acetylene-free stream passes through cooler E-108 and enters the T-103 C<sub>2</sub> splitter distillation column, which separates ethylene in stream #31, which flows into the TK-104 storage tank, from the bottom ethane gas in stream #32. The design of the T-103 distillation column is observed further in the report.

The resulting ethane stream is recycled back into the process, heated by the E-109 heat exchanger from -8.6°C to 20°C. The stream then flows through the E-110 heat exchanger, which further heats the ethane stream to 100°C. The design of the E-110 heat exchanger is observed further in the report. Finally, the pressure relief valve PRV-101 reduces the pressure of the stream to 1 bar before entering the mixer M-101.

### **2.3 Reaction Kinetics**

The kinetics of the ethane steam cracking process have been studied by a wide range of researchers. Among these, the most comprehensive and widely accepted formulations were developed by Sundaram and Froment (1977), who systematically modeled the cracking of ethane, propane, and their mixtures [38]. In their study, they discussed three kinetic models of ethylene production via steam cracking of ethane, with the implementation of the Hougen-Watson approach. Their work demonstrated that simplified schemes, namely Model III, could accurately represent complex radical systems when supported by statistical validation and regression analysis. Due to its balance between accuracy and computational simplicity, the Model III scheme was selected for process simulation and industrial reactor design. The ethane dehydrogenation reaction is accompanied by four side reactions, presented in Table 4. The rate expressions were derived for reactions R1-R5 in terms of concentrations. The extensive derivation can be seen in Appendix B. The abbreviations of compounds were used for visual simplicity, refer to the List of Abbreviations.

**Table 4.** Reaction kinetics [38]

| Reaction                                                 | Rate expressions                                         | Type |
|----------------------------------------------------------|----------------------------------------------------------|------|
| <b>R1</b><br>$C_2H_6 \leftrightarrow C_2H_4 + H_2$       | $r_1 = k_1(C_{ETH} - \frac{C_{ETLN} * C_{HRG}}{K_{C1}})$ | Main |
| <b>R2</b><br>$2C_2H_6 \rightarrow C_3H_8 + CH_4$         | $r_2 = k_2 C_{ETH}$                                      | Side |
| <b>R3</b><br>$C_3H_6 \leftrightarrow C_2H_2 + CH_4$      | $r_3 = k_3(C_{PRO} - \frac{C_{ACT} * C_{MET}}{K_{C2}})$  | Side |
| <b>R4</b><br>$C_2H_2 + C_2H_4 \rightarrow C_4H_6$        | $r_4 = k_4(C_{ACT} C_{ETLN})$                            | Side |
| <b>R5</b><br>$C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$ | $r_5 = k_5(C_{ETH} C_{ETLN})$                            | Side |

The steady-state continuity equations for each of the compounds can be formulated as follows:

$$\frac{dF_j}{dV} = - \sum_{i=1}^{N_r} s_{ji} r_i \quad (6)$$

The continuity equations are listed in Table 5. The extended derivation can be accessed in Appendix B.

**Table 5.** Continuity equations

| Compound      | Differential Mole Balance | Stoichiometric Form     |
|---------------|---------------------------|-------------------------|
| Ethane        | $dF_{ETH}/dV$             | $-r_1 - 2r_2 - r_5$     |
| Ethylene      | $dF_{ETLN}/dV$            | $r_1 + r_2 - r_4 - r_5$ |
| Hydrogen      | $dF_{HRG}/dV$             | $r_1$                   |
| Methane       | $dF_{MET}/dV$             | $2r_2 + r_3 + r_5$      |
| Propylene     | $dF_{PRLN}/dV$            | $-r_3 + r_5$            |
| Propane       | $dF_{PRO}/dV$             | $r_2$                   |
| Acetylene     | $dF_{ACT}/dV$             | $r_3 - r_4$             |
| 1,3-butadiene | $dF_{BDN}/dV$             | $r_4$                   |

The rate coefficients are expressed through an Arrhenius equation (Eq. (7)) with derived parameters presented in Table 6, with extensive derivation in Appendix B:

$$k = Ae^{\frac{Ea}{RT}} \quad (7)$$

where  $k_i$  is the rate coefficient for the  $i$ th reaction in  $\text{sec}^{-1}$  or  $\text{mol}^{-1}\text{sec}^{-1}$ ,  $A$  is the frequency factor in  $\text{sec}^{-1}$ ,  $Ea$  is the activation energy in  $\text{kcal/mol}$ ,  $R$  is the gas constant in  $\text{kcal/molK}$ , and  $T$  is the temperature in  $\text{K}$ .

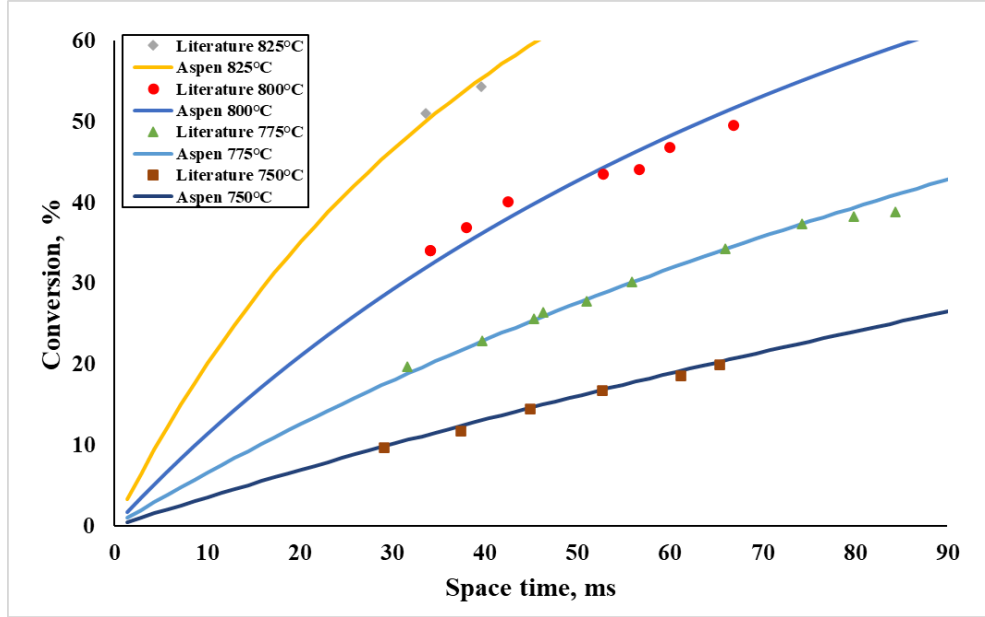
**Table 6.** Power law kinetics

|     | Reaction                                                                                     | A ( $\text{sec}^{-1}$ or $\text{mol}^{-1} \text{sec}^{-1}$ ) | Ea ( $\text{kcal/mol}$ ) |
|-----|----------------------------------------------------------------------------------------------|--------------------------------------------------------------|--------------------------|
| R1  | $\text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_4 + \text{H}_2$                         | 4.65E+13                                                     | 65.2                     |
| R2  | $2\text{C}_2\text{H}_6 \rightarrow \text{C}_3\text{H}_8 + \text{CH}_4$                       | 3.85E+11                                                     | 65.25                    |
| R3  | $\text{C}_3\text{H}_6 \rightarrow \text{C}_2\text{H}_2 + \text{CH}_4$                        | 9.81E+08                                                     | 36.92                    |
| R4  | $\text{C}_2\text{H}_2 + \text{C}_2\text{H}_4 \rightarrow \text{C}_4\text{H}_6$               | 1.03E+12                                                     | 41.26                    |
| R5  | $\text{C}_2\text{H}_4 + \text{C}_2\text{H}_6 \rightarrow \text{C}_3\text{H}_6 + \text{CH}_4$ | 7.08E+13                                                     | 60.43                    |
| R1' | $\text{C}_2\text{H}_4 + \text{H}_2 \rightarrow \text{C}_2\text{H}_6$                         | 9.91E+08                                                     | 33                       |
| R3' | $\text{C}_2\text{H}_2 + \text{CH}_4 \rightarrow \text{C}_3\text{H}_6$                        | 6.03E+04                                                     | 7.1                      |

#### 2.4 Aspen Validation of the Kinetic Model

In order to validate the kinetic model developed by Sundaram and Froment (1977), which used the experimental data from Froment (1976) [39], the paper presented the experimental results for a pilot reactor of the following dimensions: a length of 21.75 m in the reaction section and an internal diameter of 0.01 m. Mathematical calculations in Python and reaction simulations on Aspen were conducted. Specifically, the conversion of ethane against the space-time of the reactor trends obtained were compared to those provided by research.

Aspen Plus simulations were performed on PFR with the same setup as in the previous chapter. Sensitivity analysis was conducted to test the behavior of ethane conversion across all temperatures, and the length of the reactor was varied in order to change the space time of the reactor. The results and comparison between the Aspen model and experimental data are shown in Figure 7.

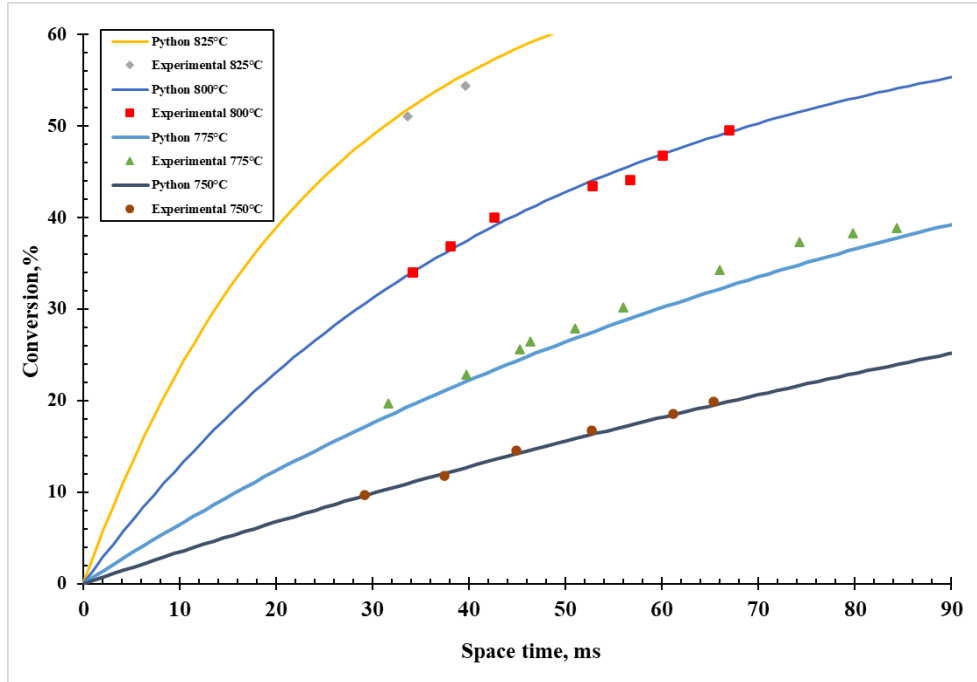


**Figure 7.** Comparison of Aspen simulations and experimental data [39]

Visually, it is noticeable that the model performs better at lower temperatures, with more correlation with experimental data. While at higher temperatures, it tends to fluctuate, though the overall resemblance of the data to the model is high.

### *2.5 Python Validation of the Kinetic Model*

Python tests were performed by solving continuity equations listed in Table 5. A system of initial value differential equations was solved using the “Runge-Kutta 45(RK45)” method in a range of reactor volumes from 0 to 1.71 L. Although temperature points of 825°C, 800°C, 775°C, and 750°C were employed to match the conditions of the reactor, the pilot reactor of the experiment did not indicate a particular temperature profile of the reactor, only the outlet temperature range of 650°C to 870°C. Hence, for a more accurate simulation for each point, the temperature was reduced to the average value to account for the reactor’s non-uniform temperature profile. The results were plotted and are shown in Figure 8.



**Figure 8.** Comparison of Python simulation and experimental data [39]

Visually, Python tests performed more consistently than Aspen simulations, with the least correlation at 775°C and 800°C. Overall, plots indicate a good resemblance, depicting a fine correlation between data and the overall trend.

In order to express similarities in data not only visually, but numerically  $R^2$  value test was performed between experimental data and Aspen or Python simulations.  $R^2$  value indicates the quality of fitting between two datasets ranges from 0 to 1, where 1 indicates a perfect fit and 0 indicates no correlation at all, with negative values suggesting to use the average values of the data, instead of fitting. Tests were performed using Python as well, and results are shown in Table 7.

**Table 7.**  $R^2$  analysis between Python, Aspen, and experimental values

|                                | <b><math>R^2</math> value</b> |        |        |        |
|--------------------------------|-------------------------------|--------|--------|--------|
| <b>Correlation/Temperature</b> | 750°C                         | 775°C  | 800°C  | 850°C  |
| <b>Python-Experimental</b>     | 0.9927                        | 0.9421 | 0.9143 | 0.9949 |
| <b>Aspen-Experimental</b>      | 0.9873                        | 0.9835 | 0.8913 | 0.9485 |

The  $R^2$  values are consistently high across all tests, with the least being at 800°C for Aspen Plus simulations and the highest between Python and Experimental values at 850°C. Strong fit is observed at temperatures of 750°C and 850°C, with  $R^2$  values being 0.9927, 0.9873

and 0.9949, and 0.9485, respectively, for Python and Aspen tests. Overall, at high temperatures, both Aspen Plus and Python show great correlation, which should be noted for further extrapolation for higher operating temperatures of our reactor (850°C).

## 2.6 Material Balance

**Table 8.** Mass balance of 1-6 streams.

| Stream                        | 1      | 2      | 3     | 4      | 5         | 6         |
|-------------------------------|--------|--------|-------|--------|-----------|-----------|
| Temperature, °C               | 25.00  | 100.00 | 25.00 | 101.54 | 95.67     | 205.27    |
| Pressure, bar                 | 1.00   | 1.00   | 1.00  | 1.00   | 1.00      | 4.00      |
| Vapor fraction                | 1.00   | 1.00   | 0.00  | 1.00   | 1.00      | 1.00      |
| Mass flow rates (kg/h)        |        |        |       |        |           |           |
| CH <sub>4</sub>               | 1026.7 | 1026.7 | 0     | 0      | 1026.7    | 1026.7    |
| C <sub>3</sub> H <sub>8</sub> | 705.54 | 705.54 | 0.00  | 0.00   | 708.01    | 708.01    |
| C <sub>2</sub> H <sub>4</sub> | 0      | 0      | 0     | 0      | 5424.5    | 5424.5    |
| C <sub>3</sub> H <sub>6</sub> | 0      | 0      | 0     | 0      | 298.11    | 298.11    |
| H <sub>2</sub>                | 0      | 0      | 0     | 0      | 0         | 0         |
| C <sub>2</sub> H <sub>6</sub> | 45706  | 45706  | 0     | 0      | 72111     | 72111     |
| H <sub>2</sub> O              | 0      | 0      | 13511 | 13511  | 13511     | 13511     |
| C <sub>2</sub> H <sub>2</sub> | 0      | 0      | 0     | 0      | 0.0017655 | 0.0017655 |
| C <sub>4</sub> H <sub>6</sub> | 0      | 0      | 0     | 0      | 0         | 0.0       |
| Total                         | 47438  | 47438  | 13511 | 13511  | 93080     | 93080     |

Table 8 describes the inlet and feed-preparation section of the process. Streams 1-6 show natural gas and water entering separately, being heated, mixed, and then compressed before entering the cracking section. At this stage, the total mass flow increases because the hydrocarbon feed is combined with steam.

**Table 9.** Mass balance of 7-12 streams.

| Stream                        | 7         | 8      | 9      | 10         | 11     | 12       |
|-------------------------------|-----------|--------|--------|------------|--------|----------|
| Temperature, °C               | 850.00    | 850.00 | 200.00 | 40.00      | 40.00  | 40.00    |
| Pressure, bar                 | 4.00      | 3.99   | 4.00   | 4.00       | 4.00   | 4.00     |
| Vapor fraction                | 1.00      | 1.00   | 1.00   | 0.00       | 1.00   | 0.01     |
| Mass flow rates (kg/h)        |           |        |        |            |        |          |
| CH <sub>4</sub>               | 1026.7    | 6828.3 | 6828.3 | 0.0066061  | 6828.3 | 0.68283  |
| C <sub>3</sub> H <sub>8</sub> | 708.01    | 1321.4 | 1321.4 | 0.00018662 | 1321.4 | 0.13214  |
| C <sub>2</sub> H <sub>4</sub> | 5424.5    | 32992  | 32992  | 0.049944   | 32992  | 3.2992   |
| C <sub>3</sub> H <sub>6</sub> | 298.11    | 882.10 | 882.10 | 0.00046035 | 882.10 | 0.08821  |
| H <sub>2</sub>                | 0         | 2656.2 | 2656.2 | 0.00047667 | 2656.2 | 0.26562  |
| C <sub>2</sub> H <sub>6</sub> | 72111     | 26216  | 26216  | 0.027250   | 26216  | 2.6216   |
| H <sub>2</sub> O              | 13511     | 13511  | 13511  | 12313      | 1198.4 | 1198.2   |
| C <sub>2</sub> H <sub>2</sub> | 0.0017655 | 331.61 | 331.61 | 0.0050882  | 331.61 | 0.033161 |
| C <sub>4</sub> H <sub>6</sub> | 0.0       | 8340.2 | 8340.2 | 0.0022397  | 8340.2 | 0.83402  |
| Total                         | 93080     | 93080  | 93080  | 12313      | 80766  | 1206.2   |

Table 9 presents the reactor outlet and initial water-removal section. Streams 7-12 show the high-temperature cracking products after the furnace, followed by cooling and quenching. In this part, ethane is strongly converted into ethylene, hydrogen, methane, and other by-products, while a large amount of water is condensed and removed.

**Table 10.** Mass balance of 13-18 streams.

| Stream                        | 13      | 14      | 15     | 16     | 17      | 18      |
|-------------------------------|---------|---------|--------|--------|---------|---------|
| Temperature, °C               | 40.00   | 99.41   | 25.00  | 40.12  | 40.00   | 75.23   |
| Pressure, bar                 | 4.00    | 10.00   | 1.00   | 1.00   | 10.00   | 15.00   |
| Vapor fraction                | 1.00    | 1.00    | 0.00   | 0.00   | 1.00    | 1.00    |
| Mass flow rates (kg/h)        |         |         |        |        |         |         |
| CH <sub>4</sub>               | 6827.6  | 6827.6  | 0      | 0      | 6827.6  | 6827.6  |
| C <sub>3</sub> H <sub>8</sub> | 1321.2  | 1321.2  | 0      | 0      | 1321.2  | 1321.2  |
| C <sub>2</sub> H <sub>4</sub> | 32989   | 32989   | 0      | 0      | 32989   | 32989   |
| C <sub>3</sub> H <sub>6</sub> | 882.01  | 882.01  | 0      | 0      | 882.01  | 882.01  |
| H <sub>2</sub>                | 2656.0  | 2656.0  | 0      | 0      | 2656.0  | 2656.0  |
| C <sub>2</sub> H <sub>6</sub> | 26214   | 26214   | 0      | 0      | 26214   | 26214   |
| H <sub>2</sub> O              | 0.11984 | 0.11984 | 159027 | 159027 | 0.11984 | 0.11984 |
| C <sub>2</sub> H <sub>2</sub> | 331.58  | 331.58  | 0      | 0      | 331.58  | 331.58  |
| C <sub>4</sub> H <sub>6</sub> | 8339.4  | 8339.4  | 0      | 0      | 8339.4  | 8339.4  |
| Total                         | 79560   | 79560   | 159027 | 159027 | 79560   | 79560   |

Table 10 shows the dehydration and first compression stage of the cracked gas. Streams 13-18 indicate that after most water is removed, the gas stream becomes much drier and is then compressed for downstream separation. This section mainly prepares the hydrocarbon-rich stream for low-temperature fractionation.

**Table 11.** Mass balance of 19-24 streams.

| Stream                        | 19      | 20      | 21      | 22      | 23      | 24      |
|-------------------------------|---------|---------|---------|---------|---------|---------|
| Temperature, °C               | 40.00   | 65.02   | -107.57 | -107.57 | -107.57 | -106.84 |
| Pressure, bar                 | 15.00   | 20.00   | 20.00   | 20.00   | 20.00   | 19.94   |
| Vapor fraction                | 1.00    | 1.00    | 0.38    | 0.00    | 1.00    | 1.00    |
| Mass flow rates (kg/h)        |         |         |         |         |         |         |
| CH <sub>4</sub>               | 6827.6  | 6827.6  | 6827.6  | 6827.6  | 0       | 6816.5  |
| C <sub>3</sub> H <sub>8</sub> | 1321.2  | 1321.2  | 1321.2  | 1321.2  | 0       | 0       |
| C <sub>2</sub> H <sub>4</sub> | 32989   | 32989   | 32989   | 32989   | 0       | 127.99  |
| C <sub>3</sub> H <sub>6</sub> | 882.01  | 882.01  | 882.01  | 882.01  | 0       | 0       |
| H <sub>2</sub>                | 2656.0  | 2656.0  | 2656.0  | 2.6560  | 2653.3  | 2.6560  |
| C <sub>2</sub> H <sub>6</sub> | 26214   | 26214   | 26214   | 26214   | 0       | 0.10764 |
| H <sub>2</sub> O              | 0.11984 | 0.11984 | 0.11984 | 0.11984 | 0       | 0       |
| C <sub>2</sub> H <sub>2</sub> | 331.58  | 331.58  | 331.58  | 331.58  | 0       | 0.19009 |
| C <sub>4</sub> H <sub>6</sub> | 8339.4  | 8339.4  | 8339.4  | 8339.4  | 0       | 0       |
| Total                         | 79560   | 79560   | 79560   | 76907   | 2653.3  | 6947.4  |

Table 11 describes the cooling and demethanizer section. Streams 19-24 show the compressed gas being cooled to cryogenic conditions and then separated in the demethanizer. In this unit, hydrogen and methane leave as the light overhead stream, while heavier C<sub>2</sub>+ components continue for further purification.

**Table 12.** Mass balance of 25-30 streams.

| Stream                        | 25      | 26     | 27      | 28     | 29         | 30         |
|-------------------------------|---------|--------|---------|--------|------------|------------|
| Temperature, °C               | -16.77  | -19.51 | 92.39   | 60.00  | 60.00      | -29.12     |
| Pressure, bar                 | 20.00   | 19.85  | 20.00   | 20.00  | 20.00      | 20.00      |
| Vapor fraction                | 0.00    | 1.00   | 0.00    | 1.00   | 1.00       | 0.00       |
| Mass flow rates (kg/h)        |         |        |         |        |            |            |
| CH <sub>4</sub>               | 11.133  | 11.133 | 0       | 0      | 11.132     | 11.132     |
| C <sub>3</sub> H <sub>8</sub> | 1321.2  | 2.4703 | 1318.8  | 0      | 2.4705     | 2.4705     |
| C <sub>2</sub> H <sub>4</sub> | 32861   | 32861  | 0       | 0      | 33039      | 33039      |
| C <sub>3</sub> H <sub>6</sub> | 882.01  | 298.11 | 583.90  | 0      | 298.11     | 298.11     |
| H <sub>2</sub>                | 0       | 0      | 0       | 38.484 | 0.00038484 | 0.00038484 |
| C <sub>2</sub> H <sub>6</sub> | 26214   | 26214  | 0       | 0      | 26405      | 26405      |
| H <sub>2</sub> O              | 0.11984 | 0      | 0.11984 | 0      | 0          | 0          |
| C <sub>2</sub> H <sub>2</sub> | 331.39  | 331.39 | 0       | 0      | 0.0033139  | 0.0033139  |
| C <sub>4</sub> H <sub>6</sub> | 8339.4  | 0      | 8339.4  | 0      | 0.0        | 0          |
| Total                         | 69959   | 59717  | 10242   | 38.484 | 59756      | 59756      |

Table 12 represents the deethanizer, acetylene removal, and feed to the C<sub>2</sub> splitter. Streams 25-30 show separation of C<sub>3</sub>+ components from the C<sub>2</sub> fraction, followed by hydrogenation of acetylene. As a result, the stream entering the C<sub>2</sub> splitter is mainly composed of ethylene and ethane, with acetylene almost fully removed.

**Table 13.** Mass balance of 31-36 streams.

| Stream                        | 31         | 32        | 33        | 34        | 35     | 36     |
|-------------------------------|------------|-----------|-----------|-----------|--------|--------|
| Temperature, °C               | -29.61     | -12.02    | 20.00     | 100.00    | 150.00 | 101.54 |
| Pressure, bar                 | 19.64      | 20.00     | 20.00     | 20.00     | 1.00   | 1.00   |
| Vapor fraction                | 1.00       | 0.00      | 1.00      | 1.00      | 1.00   | 0.97   |
| Mass flow rates (kg/h)        |            |           |           |           |        |        |
| CH <sub>4</sub>               | 11.132     | 0         | 0         | 0         | 0      | 0      |
| C <sub>3</sub> H <sub>8</sub> | 0          | 2.4705    | 2.4705    | 2.4705    | 0      | 0      |
| C <sub>2</sub> H <sub>4</sub> | 27615      | 5424.5    | 5424.5    | 5424.5    | 0      | 0      |
| C <sub>3</sub> H <sub>6</sub> | 0          | 298.11    | 298.11    | 298.11    | 0      | 0      |
| H <sub>2</sub>                | 0.00038484 | 0         | 0         | 0         | 0      | 0      |
| C <sub>2</sub> H <sub>6</sub> | 0.085470   | 26405     | 26405     | 26405     | 0      | 0      |
| H <sub>2</sub> O              | 0          | 0         | 0         | 0         | 28659  | 28659  |
| C <sub>2</sub> H <sub>2</sub> | 0.0015483  | 0.0017655 | 0.0017655 | 0.0017655 | 0      | 0      |
| C <sub>4</sub> H <sub>6</sub> | 0          | 0         | 0         | 0         | 0      | 0      |
| Total                         | 27626      | 32130     | 32130     | 32130     | 28659  | 28659  |

Table 13 describes the final ethylene purification and recycle section. Streams 31-36 show the C<sub>2</sub> splitter products, where ethylene is recovered as the main product and ethane is recycled back to the front end of the process. This table also includes the heating of the recycle stream and the water utility stream used in the exchanger network.

### Chapter 3. Major Equipment Design

#### 3.1 H-101 Reactor Design

##### 3.1.1. Reactor Description

The H-101 unit is a tubular plug flow reactor located in the radiant section of a gas-fired furnace, used for steam cracking of ethane to ethylene. As a highly endothermic process, continuous heat input is required. The furnace consists of convection and radiant zones: the feed is preheated in the convection section (500-800°C) and mixed with superheated steam, which reduces hydrocarbon partial pressure and limits coke formation. In the radiant section, direct heating raises temperatures to 700-900°C, with typical outlet temperatures of 775-885°C [40].

An operating temperature of 850°C was selected based on kinetic optimisation, with a pressure of 4 bar to balance throughput and minimize side reactions. Ethane conversion was set at 65% to optimize ethylene yield while limiting coke formation [41].

For preliminary design, the reactor was modeled as an isothermal plug flow reactor. Although real furnaces have temperature gradients, this simplification is standard due to limited data and is justified by continuous heat supply maintaining near-target temperatures along the reactor [41,42]. The extensive description of this chapter can be obtained in Appendix C and ESI.

### 3.1.2. Reactor Sizing

The reactor was sized using the residence time required to achieve the target conversion, with volumetric flow rates from Aspen Plus. Due to steam cracking, molar flow increases along the reactor, causing volumetric expansion from 17 to 29 m<sup>3</sup>/s, which was included in the design.

A multi-tube configuration with 72 parallel tubes was selected to maintain industrial gas velocities and limit pressure drop. NPS 4 pipes (ID 102.26 mm, SCH 40) were used, providing sufficient thickness and corrosion allowance (see Appendix M3). Tube length was fixed at 6.096 m, giving a total reactor volume of 3.577 m<sup>3</sup> and residence times of 0.20 s (inlet) and 0.12 s (outlet), within the typical 0.1-0.5 s range [43].

The tubes are arranged vertically with a pitch of 1.5×OD (≈0.17 m spacing). An 8×9 layout results in bundle dimensions of 1.37×1.20 m. Including clearances, the furnace cross-section is 2.2×2.0 m, and the total height is 8.1 m. These dimensions are consistent with an estimated heat duty of ~70 MW and represent a realistic industrial furnace design.

### 3.1.3. Pressure Drop

The pressure drop across the cracking coil was evaluated to ensure the selected tube design is hydraulically feasible at operating conditions. At 850°C, the flow is fully turbulent, so pressure losses are mainly due to friction along the tube, with minor losses considered negligible at this stage. Three methods were used for verification: Aspen Plus (Beggs-Brill), Excel hand calculations, and a Python model. All results were consistent, showing that the pressure drop is low compared to the 4-bar operating pressure and is acceptable for preliminary design.

**Table 14.** Comparison of pressure drop calculations

| Method                    | Model                   | Pressure drop (bar) |
|---------------------------|-------------------------|---------------------|
| Excel (hand calculations) | Darcy-Weisbach          | 0.0102              |
| Python                    | Iterative               | 0.0103              |
| Aspen Plus                | Beggs-Brill correlation | 0.0106              |

This pressure drop represents a very small fraction of the total operating pressure and therefore does not significantly influence reaction equilibrium or downstream separation performance [44]. The low hydraulic resistance confirms that the selected tube diameter and length provide an appropriate balance between residence time and flow resistance.

#### *3.1.4. Heat Duty*

The steam cracking of ethane is highly endothermic, and the required heat duty at 850°C was calculated to be approximately 70.83 MW from an overall energy balance. This heat is supplied by burners in the radiant section of the furnace. The large duty justifies the use of a radiant tubular furnace and high-temperature alloy materials to withstand sustained thermal loading.

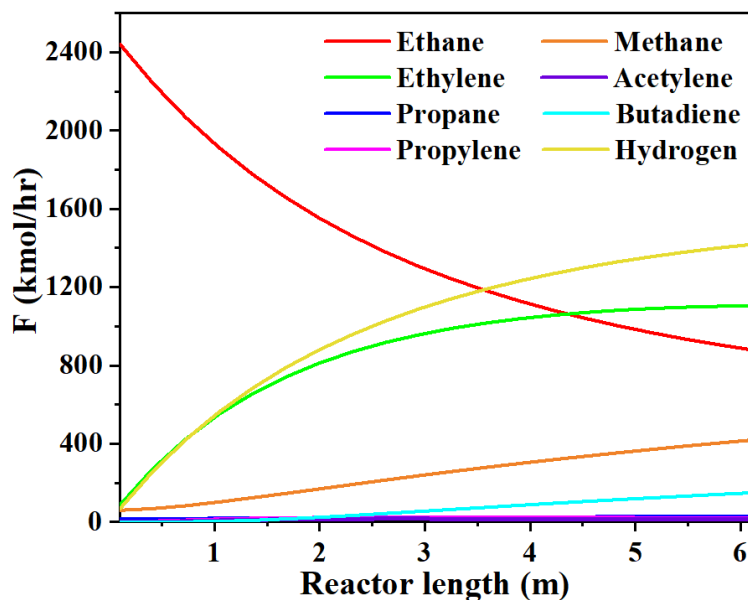
#### *3.1.5. Materials Selection*

Material selection was based primarily on high-temperature allowable stress values, creep rupture resistance, oxidation stability, and compliance with ASME elevated-temperature design standards [45]. A comparative evaluation was conducted between high-temperature stainless steels and Ni-Fe-Cr alloys specifically developed for elevated-temperature service. Using identical operating conditions, the calculated minimum wall thicknesses were 2.76 mm for Incoloy 800H [46], 2.44 mm for Type 310 stainless steel [47], and 14.88 mm for Type 309 stainless steel [48]. The significantly higher required thickness for SS 309 results from its lower allowable stress under long-term creep conditions, making it less suitable for radiant furnace service.

Although SS 310 produces a comparable thickness to 800H, thickness alone is not the governing criterion at elevated temperatures. Incoloy 800H is specifically engineered for sustained service above 800 °C, with controlled carbon content and grain structure that enhance creep rupture strength and long-term microstructural stability [49]. The final material selection of Incoloy 800H ensures compliance with elevated-temperature design standards and reflects realistic industrial practice for ethylene cracking furnace tubes.

#### *3.1.6. H-101 Final Design*

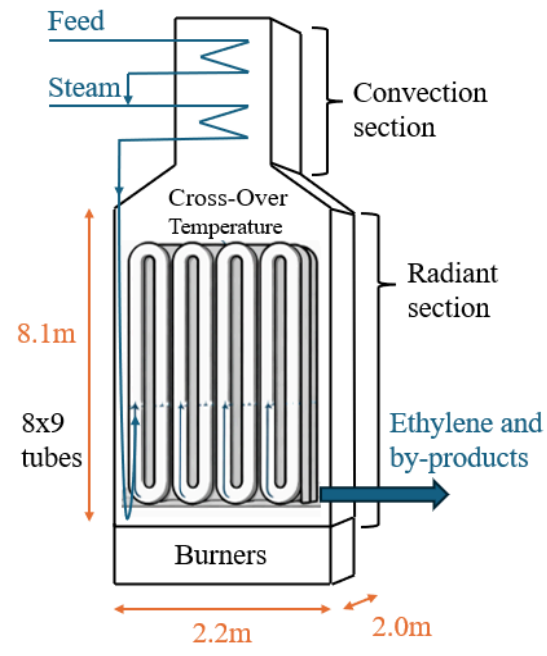
The reactants and products flow rates along the tube length were evaluated using a Sensitivity analysis in Aspen Plus. The relationships correlate with those available in literature, indicating working kinetic expression.



**Figure 9.** Compounds flow rates vs reactor length

Overall, the designed furnace satisfies the parameters of existing steam cracking furnaces worldwide according to operating conditions [43]. The schematic design and H-101 summary are presented in Table 15. The burners in industrial furnaces are located on all the tube sides and below. The sketch only showcases burners that are below the tubes for simplicity. The schematic picture was sketched manually based on the sketch presented by Tarafder, A et al (2005) [40].

**Table 15.** H-101 design specifications

| Schematic design                                                                  |     | Operating conditions                  |                            |
|-----------------------------------------------------------------------------------|-----|---------------------------------------|----------------------------|
|  |     | Temperature, °C                       | 850                        |
|                                                                                   |     | Pressure, bar                         | 4                          |
|                                                                                   |     | <b>Type and Sizing</b>                |                            |
|                                                                                   |     | Type of reactor                       | Fired furnace, Tubular PFR |
|                                                                                   |     | Selected Material                     | N08810                     |
|                                                                                   |     | Number of tubes                       | 72                         |
|                                                                                   |     | Outer diameter, mm                    | 114.3                      |
|                                                                                   |     | Inner diameter, mm                    | 102.26                     |
|                                                                                   |     | Wall thickness, mm                    | 6.02                       |
|                                                                                   |     | Length of tubes, m                    | 6.096                      |
|                                                                                   |     | Volume of the reactor, m <sup>3</sup> | 3.577                      |
| Width of reactor, m                                                               | 2.2 | Residence time, s                     | 0.12-0.2                   |
| Depth of reactor, m                                                               | 2.0 | Pressure drop, bar                    | 0.0102                     |
| Height of reactor, m                                                              | 8.1 | Heat Duty, kW                         | 70830.87                   |

### 3.2 E-105 Cooler Design

#### 3.2.1 E-105 Heat Exchanger Description

Heat exchangers are present in the system as principal units required to transfer heat between two fluids of different temperatures. The E-105 heat exchanger is a shell and tube cooler consisting of one shell pass and one tube pass. A shell and tube heat exchanger is a type of heat transfer unit where a cylindrical shell contains a bundle of round tubes with the tube axes placed parallel to the shell. Shell and tube heat exchangers consist of tubes, a shell, front- and rear-end heads, baffles, and tubesheets [50].

The hot stream flowing into E-105 is the reactor outlet after dehydration and compression at a temperature of 99°C. The hot stream is the natural gas with a composition of methane, propane, ethylene, propylene, hydrogen, ethane, water, acetylene, and butadiene, flowing into the tube side of the heat exchanger due to its high pressure of 10 bars for better efficiency of heat transfer. The water stream utilised to cool the natural gas stream flows to the shell side of the

cooler at 25°C and 1 bar. Water flows into the shell side of the heat exchanger due to its higher fouling resistance and higher fouling tendency compared to natural gas, making it easier to clean the shell-side of the heat exchanger.

### *3.2.2 E-105 Heat Exchanger Design Specifications*

Table 3 represents the design specifications of the E-105 cooler. The tube-side sizing was chosen in accordance with the Tubular Exchanger Manufacturers Association (TEMA) specifications. Based on TEMA guidelines, other variables, such as shell side design parameters, were calculated using the heat transfer equations from the Chemical Engineering Design book [51]. The natural gas and water specific heats, thermal conductivities, densities, and viscosities were chosen as the average values of these properties between the inlet and outlet temperatures, evaluated using mixture analysis in Aspen Plus (Appendix D, Table D5, D6).

The TEMA type of E-105 heat exchanger was chosen to be BEM. The bonnet type, two-pass shell, and fixed tubesheet rear-end is chosen due to the simplicity of construction and low cost, as well as for the highest value of log-mean temperature-difference factor F. In addition, a one-pass shell type allows a low pressure drop, which is characteristic of heat transfer between natural gas and water [50].

As the basis of calculations, the overall heat transfer coefficient U was assumed to be 250 W/m<sup>2</sup>°C, which was found at the intersection of the air and gas high-pressure process fluid coefficient and river, well, sea water service fluid coefficient (Appendix Z, Figure D1). The mass flow rate of natural gas and heat duty of the heat exchanger were taken from the overall process flow diagram as 79334 kg/h and 2.99E+5 W, respectively.

The natural gas velocity on the tube side was held in the range of 5-10 m/s, as assumed for vapours at high pressure, whereas the shell-side water velocity was kept in the range of 0.3-1 m/s (Appendix D, Table D2). The tube outside diameter, inside diameters, length, and wall thickness were chosen based on TEMA specifications (Appendix D, Table D1). At the same time, the Aspen Plus simulation suggested a tube count of 1768, with little deviation from the calculated tube count of 1594.

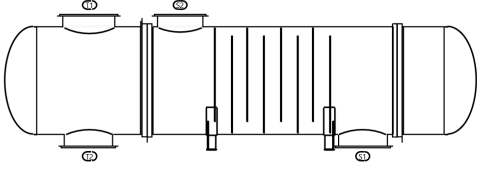
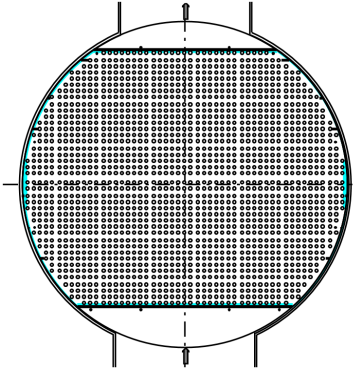
For the shell-side heat exchanger design, a 90° square pitch was chosen to accommodate high Reynolds numbers and to lower shell-side pressure drop, also allowing easier mechanical cleaning [51]. The shell diameter of 1.62 m was estimated based on the bundle diameter, which was calculated using square pitch arrangement constants for 2 tube passes (Appendix D, Table D3).

Both the heat transfer coefficient of 275.70 W/m<sup>2</sup>°C estimated from Aspen and hand calculated heat transfer coefficient of 295.01 W/m<sup>2</sup>°C exceed the initial assumed value of U. The carbon steel material was chosen based on its high thermal conductivity value of 60 W/m<sup>2</sup>°C at 40 °C (Appendix D, Figure D8).

The tube and shell side pressure drop values were estimated by hand calculations and found using Aspen Plus simulation, with little deviation and acceptable by the TEMA specifications (Appendix D, Figure D9).

The deviations of hand-calculated heat exchanger properties and Aspen Plus-derived values can be found in Appendix D, Table D9. The difference can be explained by the fact that Aspen Plus employs more detailed heat transfer correlations and temperature-dependent properties. As well as that, the simulation adjusts the parameters of the heat exchanger in the process of design implementation, calculating the velocities and heat transfer area values based on the changed input. In addition, during hand calculations, the heat transfer factors and friction factors for the shell and tube sides were manually chosen from the graphs in the Chemical Engineering Design book [51].

**Table 16.** Heat Exchanger E-105 design specifications

| Setting Plan                                                                       | Tube Layout                                                                         |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|  |  |
| TEMA Type                                                                          | BEM                                                                                 |
| In series                                                                          | 1                                                                                   |
| In parallel                                                                        | 1                                                                                   |
| Length of the tube, m                                                              | 3.66                                                                                |
| Outside diameter, mm                                                               | 0.025                                                                               |

**Table 17.** Heat Exchanger E-105 design parameters

| Design Parameters  |                 |
|--------------------|-----------------|
| Thickness, mm      | 0.0012          |
| Baffle spacing, m  | 0.24            |
| Bundle diameter, m | 1.42            |
| Shell diameter, m  | 1.62            |
| Baffle cut, %      | 25              |
| Number of tubes    | 1768            |
| Tube pattern       | 90°-square      |
| Configuration      | 1-Shell, 1-Pass |
| Type of material   | Carbon steel    |

**Table 18.** Heat Exchanger E-105 parameters

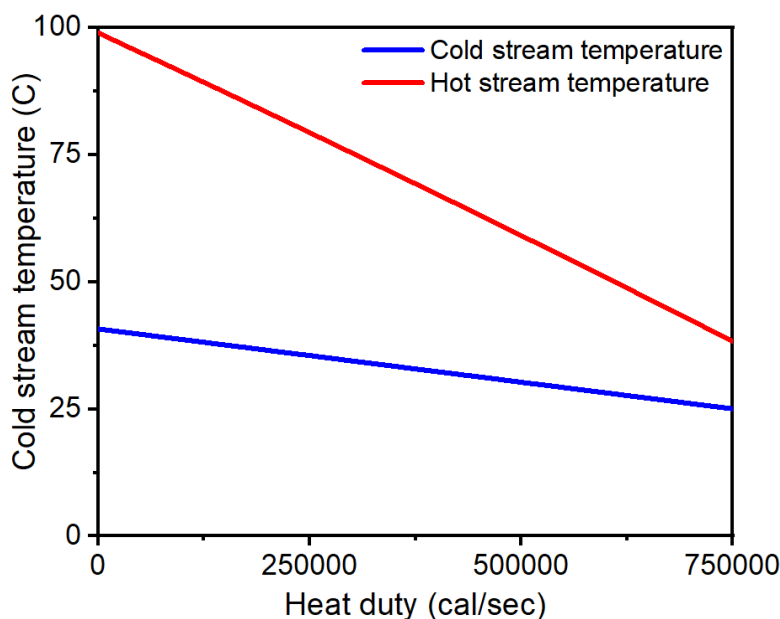
|                                          | Reactor Outlet | Water Inlet |
|------------------------------------------|----------------|-------------|
| Location                                 | Tube side      | Shell side  |
| Inlet temperature, °C                    | 99             | 25          |
| Outlet Temperature, °C                   | 40             | 40          |
| Inlet pressure, bar                      | 10             | 1           |
| Outlet pressure, bar                     | 9.9656         | 0.9760      |
| Mass flow rate, kg/hr                    | 79334.56       | 158791.63   |
| Fouling coefficients, m <sup>2</sup> K/W | 0.00025        |             |
| Heat duty, kW                            | 3156           |             |
| Heat transfer Area, m                    | 487            |             |
| Effective LMTD, C                        | 23.40          |             |

### 3.2.3 E-105 Heat Exchanger Material Selection

For the E-105 cooler, carbon steel was chosen as the construction material due to its availability, high temperature resistance, and low economic cost. Heat exchangers made of carbon steel can operate in the temperature range between 0 and 500°C, with the thermal conductivity of 60 W/m·°C at the operating conditions of 40°C (Appendix D, Figure D8). In addition, under controlled conditions, carbon steel heat exchangers are resistant to corrosion.

### 3.2.4 E-105 Heat Exchanger T-Q Curve

To assess the heat transfer efficiency of the E-105 heat exchanger, the TQ curve in Figure 10 was constructed. The graph indicates a moderate temperature gradient, which suggests an efficient heat transfer process.



**Figure 10.** E-105 Heat Exchanger T-Q Curve

## 3.3 E-110 Heater Design

### 3.3.1 E-110 Heat Exchanger Description

E-109 heat exchanger is a heater which heats the recycle stream from the C<sub>2</sub> splitter. It provides the required heat for the stream to match a feed mixer. To avoid heat loss in a mixer, the stream needs to be heated up, from -8 °C to 100 °C.

In order to reach such a steep heating, it was necessary to divide the process into two exchangers:

- 1st heat exchanger: heating from -8 °C vapor-liquid mixture to 20 °C gas, with room temperature water.
- 2nd heat exchanger: heating the gas mixture from 20°C to 100°C, with high pressure water at 150°C.

The primary objective was to minimise pressure drop across the heat exchangers and ensure the designs align with TEMA standards. The second heat exchanger is considered a major unit, while the first one is a minor unit. Physical properties for each stream are considered for mean temperatures of each stream and can be considered as operating conditions.

### *3.3.2 E-110 Heat Exchanger Design Specifications*

The design specifications for the E-110 heater are given in Table 19. Dimensions of the tube and shell were assigned according to the TEMA. Further parameters were calculated according to the Chemical Engineering Design book by Towler and Sinnott [51].

The design of this heat exchanger follows the same principles outlined in Section 2.2, where similar configurations and pressure drop considerations were discussed. However, due to different composition of the process fluid, values assumed for and associated with further calculations were different.

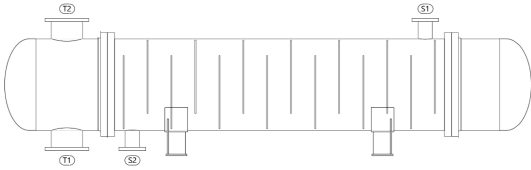
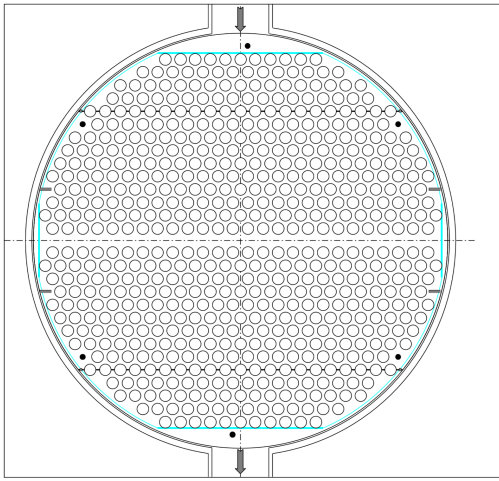
The E-110 cooler design utilizes a TEMA BEM configuration, incorporating a bonnet-type head and a fixed tubesheet rear-end. Based on an initial assumed heat transfer coefficient  $U$  of 413 W/m<sup>2</sup>°C, the unit was designed to handle a gas mass flow rate of 31904 kg/h and a total heat duty of 1495507 W.

Operating parameters were set to maintain natural gas velocities between 5 and 10 m/s and shell-side water velocities between 0.3 and 1 m/s. Mechanical specifications include a calculated tube count of 420, arranged in a 2 tube-pass configuration. The shell-side geometry features a 0.66 m diameter and a 30° triangular pitch for higher heat-transfer rates [51].

Carbon steel was selected as the material of construction, providing a thermal conductivity of 58 W/m°C at 100 °C. Final performance assessments yielded a simulated heat transfer coefficient of 427.48 W/m<sup>2</sup>°C and a manual calculation of 416.10 W/m<sup>2</sup>°C. Both tube and shell-side pressure drops were verified with TEMA standards.

The deviations of hand-calculated heat exchanger properties and Aspen Plus-derived values can be found in Appendix D, Table D10.

**Table 19.** Heat Exchanger E-110 design specifications

| Setting Plan                                                                      | Tube Layout                                                                        |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| TEMA Type                                                                         | <b>BEM</b>                                                                         |
| In series                                                                         | 1                                                                                  |
| In parallel                                                                       | 1                                                                                  |
| <b>Design Parameters</b>                                                          |                                                                                    |
| Length of the tube, m                                                             | 2,44                                                                               |
| Outside diameter, mm                                                              | 19                                                                                 |
| Thickness, mm                                                                     | 1,7                                                                                |
| Baffle spacing, m                                                                 | 0,17                                                                               |
| Bundle diameter, m                                                                | 0.55                                                                               |
| Shell diameter, m                                                                 | 0.66                                                                               |
| Baffle cut, %                                                                     | 25                                                                                 |
| Number of tubes                                                                   | 420                                                                                |
| Tube pattern                                                                      | 30-Triangular                                                                      |
| Configuration                                                                     | 1-Shell, 1-Pass                                                                    |
| Type of material                                                                  | Carbon Steel                                                                       |

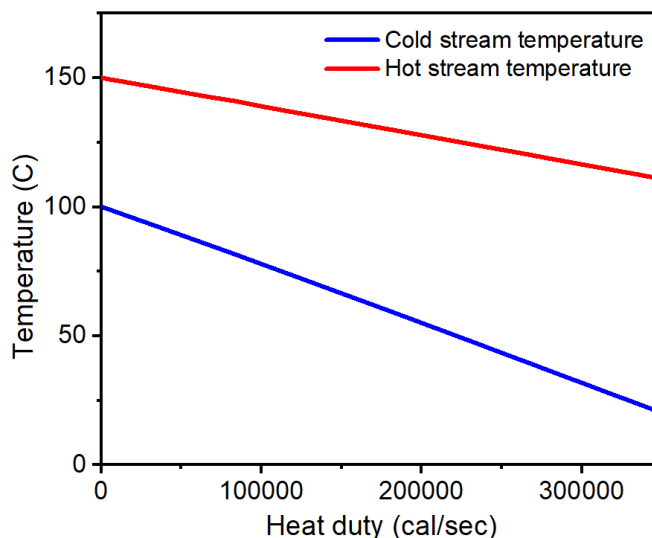
**Table 20.** Heat Exchanger E-110 parameters

|                                          | <b>C<sub>2</sub> splitter outlet</b> | <b>Water Inlet</b> |
|------------------------------------------|--------------------------------------|--------------------|
| Location                                 | Tube Side                            | Shell side         |
| Inlet temperature, C                     | 20                                   | 150                |
| Outlet Temperature, C                    | 100                                  | 110                |
| Inlet pressure, bar                      | 20                                   | 5                  |
| Outlet pressure, bar                     | 19.90                                | 4.96               |
| Mass flow rate, kg/hr                    | 31904                                | 28659              |
| Fouling coefficients, m <sup>2</sup> K/W | 0.00025                              |                    |
| Heat duty, W                             | 1495507                              |                    |
| Heat transfer Area, m <sup>2</sup>       | 61.24                                |                    |
| Effective LMTD, C                        | 59.13                                |                    |

### 3.3.3 E-110 Heat Exchanger Material Selection

For the E-110 heater, carbon steel was selected as the material of construction. This material provides a thermal conductivity of 58 W/m°C at the operating temperature of 100°C. The design accommodates a permissible service temperature range of 0 to 500°C.

### 3.3.4 E-110 Heat Exchanger T-Q Curve



**Figure 11.** E-110 Heat Exchanger T-Q Curve

For heat transfer efficiency assessment of the E-105 heat exchanger, the T-Q curve in Figure 11 was constructed. It implies an optimal temperature gradient, which in turn illustrates sufficient design of the heat exchanger.

### 3.4 T-101 Distillation Column Design

The working principle of the distillation column is to separate a mixture of two or more components that have different boiling points. The component with higher boiling point will go to the bottom stream, while the component with lower point will be distilled due to faster evaporation. The reboiler in the distillation column heats and vaporizes the liquid mixture from bottoms, while the condenser removes heat by turning the vapor into liquid from the distillates [52]. Reflux is the mixture that is returned from the condenser.

First, before the demethanizer, the hydrogen is removed from the components. For the separation of desired components, the light key and heavy key between the feed components should be chosen. They are needed for establishing the relative volatilities under column operating conditions. The boiling points at standard conditions are the following: -89°C for ethane, -104°C for ethylene, -253°C for hydrogen, -42°C for propane, -83°C for acetylene, -161°C for methane, -4.41°C for 1,3-butadiene, -48°C for propylene, and 100°C for water [53-55]. All calculations described below are performed in an Excel file (ESI).

The material for the all columns was selected Stainless Steel (SS) 316L because of its operating temperature range and corrosion resistance [56]. The selection of material is essential for the calculation of wall thicknesses and corrosion allowance. For SS 316L, the maximum

allowable stress at minimum available value of 100°F (37.8°C) was taken, and substituted 20 ksi (1379 bar). The material is prone to corrosion, therefore the corrosion rate is considered to be zero. The assumption that the welds will be fully radiographed is made, so the weld quality factor is equal to 1. Design pressure is 10% above the operating pressure [51]. For safety consideration, the obtained value of thickness was rounded up to a higher number. The wall thickness  $t$  is calculated as:

$$t = \frac{PD}{2SE - 1.2P} \quad (8)$$

where,  $P$  is the design pressure,  $D$  is the diameter of the column,  $S$  is the maximum allowable stress, and  $E$  is the weld quality factor.

The T-101 distillation column, named demethanizer, is used to separate methane to the distillate from the rest of the multicomponent feed. The purpose is to make the composition of the stream at bottoms without the mentioned component that contribute to purity of ethylene at the final stream.

The packed bed distillation column type was chosen for the T-101 unit design. To generate the design of the stages and packed internals, the type of packing should be identified for the calculation of the diameters, height of packing, and results of the hydraulic plots for the stages. The Pall rings of 38 mm size were chosen for the design since the pressure drop for the flooding is around 1.5 in H<sub>2</sub>O/ft, which is the optimal value for operation [57].



**Figure 12.** 38 mm Pall rings [58]

The flooding pressure change is calculated by the following equation:

$$\Delta P_{flood} = 0.115 F_p^{0.7} \quad (9)$$

where,  $F_p$  is the packing factor, individual for each type of packing.

The operating conditions for the T-101 distillation column are based on the boiling and dew temperatures. The feed is entered to demethanizer at -108°C, and the operating pressure is

20 bar. The distillate is separated at dew temperature of the top products at -107°C and 20 bars, while the bottoms are extracted at -17°C and 20 bars.

For the calculation of relative volatilities, the K values from Flash 2 separators in Aspen were used with distillate at dew temperature and bottoms at boiling temperature. The application of Antoine coefficients is not applied due to the diversity of compounds that are distilled through the column with varying temperatures. The equation for calculation the relative volatility is as follows:

$$\alpha_i = \frac{K_{LK}}{K_{HK}} \quad (10)$$

where,  $\alpha_i$  is the relative volatility of component i with respect to reference component,  $K_{LK}$  and  $K_{HK}$  are the K values of the light key and heavy key components.

The relative volatilities  $\alpha_{top}$  for distillate and  $\alpha_{bottom}$  for bottom were calculated separately, and the mean relative volatility  $\alpha_{ij}$  is calculated as:

$$\alpha_{ij} = \sqrt{\alpha_{top} \alpha_{bottom}} \quad (11)$$

Table 21 demonstrated the estimated relative volatilities for each compound.

**Table 21.** Estimated relative volatilities of T-101

| Compound                      | Relative volatility, $\alpha_{ij}$ |
|-------------------------------|------------------------------------|
| C <sub>2</sub> H <sub>6</sub> | 0.572                              |
| C <sub>2</sub> H <sub>4</sub> | 1.000                              |
| H <sub>2</sub>                | 0                                  |
| C <sub>3</sub> H <sub>8</sub> | 0.091                              |
| C <sub>2</sub> H <sub>2</sub> | 0.617                              |
| CH <sub>4</sub>               | 7.369                              |
| C <sub>4</sub> H <sub>6</sub> | 0.017                              |
| C <sub>3</sub> H <sub>6</sub> | 0.118                              |
| H <sub>2</sub> O              | 0.005                              |

It can be noticed from the values that from the distillate products, the methane is the light key, being the only distillate, and among bottoms the ethylene selected as heavy key having the highest value compared to other heavier fractions.

For the primary calculations of design parameters, the Fenske-Underwood-Gilliland (FUG) method was used for multicomponent feed. From this method, the minimum and actual number of stages, reflux ratio and stages above feed were calculated. The minimum number of stages were calculated using the Fenske equation:

$$N_{min} = \frac{\log[(x_{LK}/x_{HK})_D / (x_{LK}/x_{HK})_B]}{\log(\alpha_{ij})} \quad (12)$$

where,  $x_{LK}$  and  $x_{HK}$  is the light key and heavy key molar fractions, and D and B refer to distillate and bottom stream, relatively.

From the Underwood correlation, the  $\theta$  value is calculated, which is applied for further calculation of minimum reflux ratio:

$$\sum \frac{\alpha_{ij} x_{i,F}}{\alpha_{ij} - \theta} = 1 - q \quad (13)$$

where,  $q$  is the quality,  $x_{i,F}$  is the molar fraction of each component in the feed. The quality of the feed was calculated using the following formula for subcooled liquid:

$$q = \frac{C_{pV}(T_d - T_F)}{\Delta H^{vap}} \quad (14)$$

where,  $C_{pV}$  is the molar heat capacity for vapor,  $\Delta H^{vap}$  is the molar enthalpy from bubble to the dew point, and  $T_d$ ,  $T_F$  are the dew point and feed temperature of the feed stream, respectively. These values were obtained using the mixture analysis in Aspen for the inlet stream of the column.

The Underwood correlation is also used to obtain the value of minimum reflux ratio:

$$\sum \frac{\alpha_{ij} x_{i,D}}{\alpha_{ij} - \theta} = R_{min} + 1 \quad (15)$$

where,  $x_{i,D}$  is the molar fraction of given component in distillate, and  $R_{min}$  is the minimum reflux ratio.

The reflux  $R$  was estimated according to heuristics for towers, where the economically optimum reflux ratio is in the range of 1.2 - 1.5 times minimum reflux ratio [59], and shown as:

$$R = 1.2 R_{min} \quad (16)$$

The Gilliland correlation is applied for the number of stages estimation:

$$\frac{R - R_{min}}{R + 1} = \Psi \quad (17)$$

where,  $\Psi$  is the special coefficient used for calculation of stages. After identification of this value, the number of stages can be estimated from:

$$\frac{N - N_{min}}{N + 1} = 1 - \exp\left(\frac{1+54.4\Psi}{11+117.2\Psi} \times \frac{\Psi-1}{\Psi^{0.5}}\right) \quad (18)$$

where,  $N$  is the number of stages.

For estimation the feed stage location, the Kirkbride's equation is used to identify the stages above feed:

$$\frac{m}{p} = \left[ \left(\frac{B}{D}\right) \left(\frac{x_{HK}}{x_{LK}}\right)_F \left(\frac{x_{LK,B}}{x_{HK,D}}\right)^2 \right]^{0.206} \quad (19)$$

where,  $m$  is the number of stages above the feed plate,  $p$  is the number of stages below the feed.

The total number of stages  $N$  is identified as:

$$N = m + p \quad (20)$$

The further design includes the calculation of diameter and height of the column. The procedure includes the determination of column liquid - vapor factor [60].

$$F_{LV} = \left(\frac{L_W^*}{V_W^*}\right) \sqrt{\frac{\rho_V}{\rho_L}} \quad (21)$$

where,  $F_{LV}$  is the column liquid-vapor factor,  $L_W^*$  and  $V_W^*$  is the liquid and gas mass flow rate per unit cross-sectional area,  $\rho_V$  and  $\rho_L$  are the vapor and liquid densities [61].

The velocity of vapor flooding  $u_{vf}$  is required for the estimation of column diameter:

$$u_{vf} = \frac{F_c}{F_p^{0.5} \left(\frac{\rho_V}{\rho_L - \rho_V}\right)^{0.5} v_L^{0.05}} \quad (22)$$

where,  $F_c$  is the capacity parameter,  $F_p$  is the packing parameter,  $v_L$  is the kinematic viscosity of liquid.

From this, the column diameter is calculated as:

$$D_c = \sqrt{\frac{4\hat{V}_W}{f u_{vf} \pi \rho_V}} \quad (23)$$

where,  $f$  is the flooding assumed as 0.8,  $D_c$  is the column diameter,  $\hat{V}_w$  is the maximum vapor rate.

Finally, the height of the column is estimated according to HETP value that depends on the packing type. For Pall rings the value is 0.4 m [62].

$$H = HETP \times N \quad (24)$$

where, HETP is the height equivalent to the theoretical plate, and  $H$  is the column height.

For the design in Aspen, the boilup ratio was calculated theoretically as:

$$V_B = \frac{V_{m+1}}{B} \quad (25)$$

where,  $V_B$  is the boilup ratio, and  $V_{m+1}$  is the vapor in the  $(m+1)$  plate.

To account for the efficiency of the column, the O'Connell correlation was used:

$$E_0 = 51 - 32.5 \log(\mu_f \alpha_f) \quad (26)$$

where,  $E_0$  is the column efficiency,  $\mu_f$  is the molar liquid viscosity at feed stage, and  $\alpha_f$  is the relative volatility calculated at feed stage [51].

From this, the real number of stages was calculated from the equation:

$$E_0 = \frac{\text{number of ideal stages}}{\text{number of real stages}} \quad (27)$$

The theoretical values from the FUG method were placed in the DSTWU unit in Aspen for comparison. The stated number of stages is 23. Table 22 shows the results between calculated and Aspen parameters for the T-101 column.

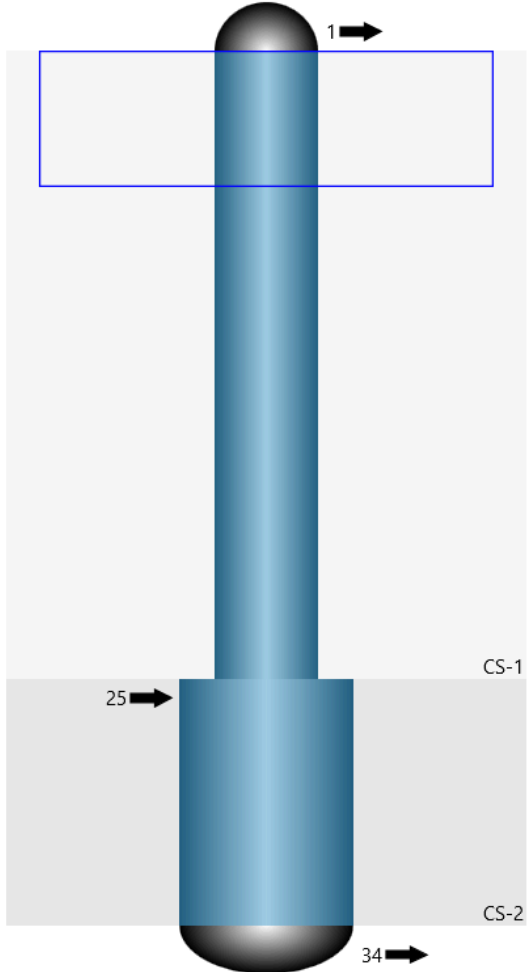
To verify whether the selected operating conditions are optimal, sensitivity analyses for reflux ratio and feed stage were performed; the results for columns T-101, T-102, and T-103 are presented in the Appendix E.

**Table 22.** Comparison of calculated and received Aspen values T-101

| Parameter                | Calculated | DSTWU Aspen |
|--------------------------|------------|-------------|
| Minimum Number of stages | 11         | 12          |
| Reflux Ratio             | 3.205      | 1.030       |
| Feed stage               | 16         | 11          |

The values show some difference in reflux ratio, and few stages difference for number of stages, which shows good correlation between data. These values were implemented for further design in RadFrac columns in Aspen. Table 23 shows the final parameters and specifications for the T-101 column.

**Table 23.** Design parameters for T-101 distillation column

| T-101 Demethanizer (Danel, Ulan)                                                   |         |                                                      |                      |
|------------------------------------------------------------------------------------|---------|------------------------------------------------------|----------------------|
| Scheme                                                                             |         | Specification details                                |                      |
|  |         | Feed flow rate, kmol/hour                            | 2692.4               |
|                                                                                    |         | Distillate flow rate, kmol/hour                      | 430.79               |
|                                                                                    |         | Bottoms flow rate, kmol/hour                         | 2261.6               |
|                                                                                    |         | Feed Phase                                           | Liquid               |
|                                                                                    |         | Calculation type                                     | Equilibrium          |
|                                                                                    |         | Condenser type                                       | Partial vapor        |
|                                                                                    |         | Reboiler type                                        | Kettle               |
|                                                                                    |         | Reflux ratio                                         | 3.2054               |
|                                                                                    |         | Number of stages                                     | 34                   |
|                                                                                    |         | Feed stage                                           | 25                   |
|                                                                                    |         | Internal type                                        | Packed               |
|                                                                                    |         | Packing                                              | Pall ring            |
|                                                                                    |         | Packing surface area, m <sup>2</sup> /m <sup>3</sup> | 139.40               |
|                                                                                    |         | Column height, m                                     | 12.8                 |
|                                                                                    |         | Column diameter, m                                   | 1.2461               |
|                                                                                    |         | Packing size                                         | 38 mm                |
|                                                                                    |         | Material                                             | Stainless steel 316L |
|                                                                                    |         | Wall thickness, mm                                   | 17                   |
|                                                                                    |         | Column efficiency, %                                 | 67                   |
| Operating conditions                                                               |         |                                                      |                      |
| Stream                                                                             | Feed    | Distillate                                           | Bottom               |
| Temperature, °C                                                                    | -108    | -107                                                 | -17                  |
| Pressure, bar                                                                      | 20      | 19.94                                                | 20                   |
| Condenser energy                                                                   |         | Reboiler energy                                      |                      |
| Heat duty, MW                                                                      | -2.1856 | Heat duty, MW                                        | 7.2875               |

### 3.5 T-102 Distillation Column Design

T-102 distillation column, also called de-ethanizer is needed to separate  $C_3+$  components to the bottom stream and  $C_2+$  components as distillate for further separation in order to increase the purity of the final ethylene product. The selection of the column type followed the same process as in the T-101 unit. As a result, 38 mm metal Pall rings were selected for the design. The operating temperature ranges from  $-16.8^{\circ}\text{C}$  to  $92^{\circ}\text{C}$ , and pressure is 20 bars. The distillate is separated at  $-20^{\circ}\text{C}$ , while the bottoms are extracted at  $92^{\circ}\text{C}$  both at 20 bars. Based on the boiling points, ethane is LK, and propylene is HK.  $C_2H_4$ ,  $H_2$ ,  $C_2H_2$ ,  $CH_4$  have lower boiling points and will evaporate easier, while  $H_2O$ ,  $C_4H_6$ ,  $C_3H_8$  have higher boiling points and will go to bottoms. For relative volatilities, K values from Flash 2 separators were used and applied according to Eq.10 and 11. The outcomes are presented in Table 24.

**Table 24.** Estimated relative volatilities of T-102

| Compound | Relative volatility, $\alpha_{ij}$ |
|----------|------------------------------------|
| $C_2H_6$ | 2.001                              |
| $C_2H_4$ | 2.568                              |
| $H_2$    | 0                                  |
| $C_3H_8$ | 0.877                              |
| $C_2H_2$ | 2.320                              |
| $CH_4$   | 5.902                              |
| $C_4H_6$ | 1.383                              |
| $C_3H_6$ | 1.000                              |
| $H_2O$   | 1.207                              |

Design parameters for multicomponent feed were calculated using the FUG method. This approach was used to calculate the reflux ratio, the minimal and actual number of stages, and the stages above the feed using equations 5-15. Table 24 shows the results between calculated and Aspen parameters for the T-102 column. All values are presented in Table 26.

**Table 25.** Comparison of calculated and received Aspen values T-102

| Parameter                | Calculated | DSTWU Aspen |
|--------------------------|------------|-------------|
| Minimum Number of stages | 20         | 23          |
| Reflux Ratio             | 0.965      | 0.822       |
| Feed stage               | 26         | 24          |

**Table 26.** Design parameters for T-102 distillation column

| T-102 De-ethanizer (Danel) |        |                                                      |                      |
|----------------------------|--------|------------------------------------------------------|----------------------|
| Scheme                     |        | Specification details                                |                      |
|                            |        | Feed flow rate, kmol/hour                            | 2261.6               |
|                            |        | Distillate flow rate, kmol/hour                      | 2063.7               |
|                            |        | Bottoms flow rate, kmol/hour                         | 197.96               |
|                            |        | Feed Phase                                           | Liquid               |
|                            |        | Calculation type                                     | Equilibrium          |
|                            |        | Condenser type                                       | Partial vapor        |
|                            |        | Reboiler type                                        | Kettle               |
|                            |        | Reflux ratio                                         | 0.96542              |
|                            |        | Number of stages                                     | 48                   |
|                            |        | Feed stage                                           | 26                   |
|                            |        | Internal type                                        | Packed               |
|                            |        | Packing                                              | Pall ring            |
|                            |        | Packing surface area, m <sup>2</sup> /m <sup>3</sup> | 139.40               |
|                            |        | Column height, m                                     | 25                   |
|                            |        | Column diameter, m                                   | 1.8                  |
|                            |        | Packing size                                         | 38 mm                |
|                            |        | Material                                             | Stainless steel 316L |
|                            |        | Wall thickness, mm                                   | 20                   |
|                            |        | Column efficiency, %                                 | 74                   |
| Operating conditions       |        |                                                      |                      |
| Stream                     | Feed   | Distillate                                           | Bottom               |
| Temperature, °C            | -16.8  | -20                                                  | 92                   |
| Pressure, bar              | 20     | 19.8                                                 | 20                   |
| Condenser energy           |        | Reboiler energy                                      |                      |
| Heat duty, MW              | -5.365 | Heat duty, MW                                        | 11.475               |

### 3.6 T-103 Distillation Column Design

Distillation column T-103 is the C<sub>2</sub> Splitter with the feed coming from the deethanizer's distillate product with the C<sub>2</sub>H<sub>4</sub> distilled on top and C<sub>2</sub>H<sub>6</sub> going to the bottoms. The main desired parameter from this column is the 99.9% purity of the ethylene. Based on the boiling points, the LK is ethylene, and the HK is ethane. The same procedure was done in choosing the type of column as in the T-101 unit. Therefore, the Pall rings of 38mm size were chosen for the design. Operating conditions of T-103 are 20 bar pressure and temperature range is -29.6°C to -12°C. The distillate product leaves the column at -29.6°C and 20 bar, bottom product at -12°C and 20 bar. For the calculation of relative volatilities, the K values from Flash 2 separators were used with distillate at dew temperature and bottoms at boiling temperature by equations 2, 3. The results are shown in Table 27.

**Table 27.** Estimated relative volatilities of T-103

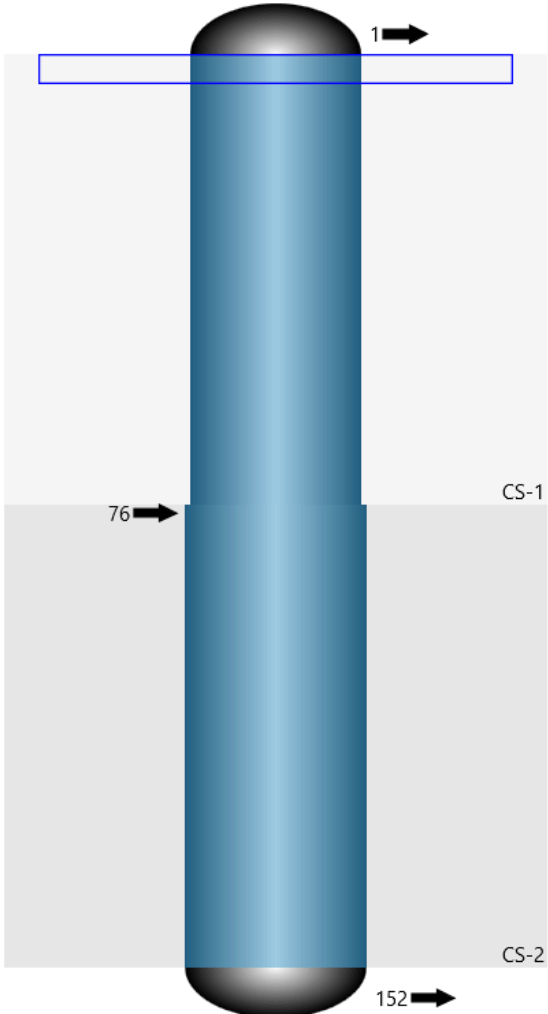
| Compound                      | Relative volatility, $\alpha_{ij}$ |
|-------------------------------|------------------------------------|
| C <sub>2</sub> H <sub>6</sub> | 1.000                              |
| C <sub>2</sub> H <sub>4</sub> | 1.453                              |
| H <sub>2</sub>                | 0                                  |
| C <sub>3</sub> H <sub>8</sub> | 0.290                              |
| C <sub>2</sub> H <sub>2</sub> | 0                                  |
| CH <sub>4</sub>               | 5.069                              |
| C <sub>4</sub> H <sub>6</sub> | 0                                  |
| C <sub>3</sub> H <sub>6</sub> | 0.355                              |
| H <sub>2</sub> O              | 0                                  |

The FUG method was used for the initial calculations of design parameters concerning multicomponent feed. Using this method, the minimum and actual stage numbers, reflux ratio, and stages exceeding the feed were determined, equations 5-15. The values presented in Table 28.

**Table 28.** Comparison of calculated and received Aspen values T-103

| Parameter                | Calculated | DSTWU Aspen |
|--------------------------|------------|-------------|
| Minimum Number of stages | 61         | 61          |
| Reflux Ratio             | 4.6961     | 4.3706      |
| Feed stage               | 64         | 67          |

**Table 29.** Design parameters for T-103 distillation column

| T-103 C <sub>2</sub> Splitter (Ulan)                                               |         |                                                      |                      |
|------------------------------------------------------------------------------------|---------|------------------------------------------------------|----------------------|
| Scheme                                                                             |         | Specification details                                |                      |
|  |         | Feed flow rate, kmol/hour                            | 2063.7               |
|                                                                                    |         | Distillate flow rate, kmol/hour                      | 985.04               |
|                                                                                    |         | Bottoms flow rate, kmol/hour                         | 1078.6               |
|                                                                                    |         | Feed Phase                                           | Liquid               |
|                                                                                    |         | Calculation type                                     | Equilibrium          |
|                                                                                    |         | Condenser type                                       | Partial vapor        |
|                                                                                    |         | Reboiler type                                        | Kettle               |
|                                                                                    |         | Reflux ratio                                         | 5.469                |
|                                                                                    |         | Number of stages                                     | 128                  |
|                                                                                    |         | Feed stage                                           | 64                   |
|                                                                                    |         | Internal type                                        | Packed               |
|                                                                                    |         | Packing                                              | Pall ring            |
|                                                                                    |         | Packing surface area, m <sup>2</sup> /m <sup>3</sup> | 139.40               |
|                                                                                    |         | Column height, m                                     | 60                   |
|                                                                                    |         | Column diameter, m                                   | 2.5                  |
|                                                                                    |         | Packing size                                         | 38 mm                |
|                                                                                    |         | Material                                             | Stainless steel 316L |
|                                                                                    |         | Wall thickness, mm                                   | 24                   |
|                                                                                    |         | Column efficiency, %                                 | 84                   |
| Operating conditions                                                               |         |                                                      |                      |
| Stream                                                                             | Feed    | Distillate                                           | Bottom               |
| Temperature, °C                                                                    | -29     | -29.6                                                | -12                  |
| Pressure, bar                                                                      | 20      | 19.6                                                 | 20                   |
| Condenser energy                                                                   |         | Reboiler energy                                      |                      |
| Heat duty, MW                                                                      | -13.697 | Heat duty, MW                                        | 16.678               |

## Chapter 4. Minor Equipment Design

### 4.1 Heating and Cooling Units

The heat duty of a heat exchanger can be calculated using the following formula [51]:

$$Q = n \times C_p \times \Delta T \quad (28)$$

where,

Q - heat duty, kW

n - molar flow rate, kmol/s

C<sub>p</sub> - heat capacity of mixture, J/kmol°C

ΔT - temperature difference, °C

#### 4.1.1 Heater E-101

Heater E-101 is used to heat the inlet natural gas stream #1 from 25°C to 100°C. The operating pressure is 1 bar. The heat duty is calculated according to Equation 28.

**Table 30.** Input data for E-101 heat duty calculation

| Inlet T,<br>°C | Outlet T,<br>°C | n, kmol/s | C <sub>p</sub> at T = 75°C,<br>kJ/kmol°C | Calculated Q,<br>kW | Aspen Plus<br>Derived Q, kW |
|----------------|-----------------|-----------|------------------------------------------|---------------------|-----------------------------|
| 25             | 100             | 0.4444    | 59.93                                    | 1930.92             | 1893.15                     |

#### 4.1.2 Heater E-102

Heater E-102 is used to heat the inlet water stream #3 from 25°C to 100°C. The operating pressure is 1 bar. Since a phase change from liquid to vapour phase occurs, the heat duty is calculated as follows [51]:

$$Q = n \times \Delta H \quad (29)$$

where,

Q - heat duty, kW

n - molar flow rate, kmol/s

ΔH - enthalpy change, kJ/mol

**Table 31.** Input data for E-102 heat duty calculation

| Inlet T, °C | Outlet T, °C | n, kmol/s | $\Delta H$ at T = 25°C, kJ/kmol | $\Delta H$ at T = 100°C, kJ/mol | Calculated Q, kW | Aspen Plus Derived Q, kW |
|-------------|--------------|-----------|---------------------------------|---------------------------------|------------------|--------------------------|
| 25          | 100          | 0.2083    | -287741                         | -239302                         | 10298.14         | 10091.4                  |

#### 4.1.3 Heater E-103

Heater E-103 is used to heat the compressed mixed feed stream #6 from 214°C to 680°C. The operating pressure is 4 bar. The heat duty is calculated according to Equation 28.

**Table 32.** Input data for E-103 heat duty calculation

| Inlet T, °C | Outlet T, °C | n, kmol/s             | $C_p$ at T = 447°C, kJ/kmol°K | Calculated Q, kW | Aspen Plus Derived Q, kW |
|-------------|--------------|-----------------------|-------------------------------|------------------|--------------------------|
| 214         | 680          | 0.9523966<br>65781899 | 83.92                         | 36877.64         | 37898.15382140<br>4      |

#### 4.1.4 Cooler E-104

Cooler E-104 is used to cool the hot product stream #8 from 850°C to 200°C. The operating pressure is 4 bar. The heat duty is calculated according to Equation 28.

**Table 33.** Input data for E-104 heat duty calculation

| Inlet T, °C | Outlet T, °C | n, kmol/s            | $C_p$ at T = 525°C, kJ/kmol°K | Calculated Q, kW | Aspen Plus Derived Q, kW |
|-------------|--------------|----------------------|-------------------------------|------------------|--------------------------|
| 850         | 200          | 1.3219480<br>6924322 | 65.35                         | -55828.18        | -57266.0212845<br>59996  |

#### 4.1.5 Cooler E-106

Cooler E-106 is used to cool the compressed gas stream #18 from 79°C to 40°C. The operating pressure is 15 bar. The heat duty is calculated according to Equation 28.

**Table 34.** Input data for E-106 heat duty calculation

| Inlet T, °C | Outlet T, °C | n, kmol/s            | Cp at T = 59.5°C, kJ/kmolK | Calculated Q, kW | Aspen Plus Derived Q, kW |
|-------------|--------------|----------------------|----------------------------|------------------|--------------------------|
| 79          | 40           | 1.1135042<br>2595332 | 45.69                      | -1970.61         | -1781.49187408<br>32     |

*4.1.6 Cooler E-107*

Cooler E-107 is used to cool the compressed gas stream #20 from 65°C to -108°C. The operating pressure is 20 bar. The heat duty is calculated according to Equation 28.

**Table 35.** Input data for E-107 heat duty calculation

| Inlet T, °C | Outlet T, °C | n, kmol/s            | Cp at T = 30°C, kJ/kmol·K | Calculated Q, kW | Aspen Plus Derived Q, kW |
|-------------|--------------|----------------------|---------------------------|------------------|--------------------------|
| 65          | -108         | 1.1135042<br>2595332 | 45.14                     | -3494.42         | -16891.7930639<br>28     |

*4.1.7 Cooler E-108*

Cooler E-108 is used to cool the acetylene-free C<sub>2</sub> stream #27 from 60°C to -29.12°C. The operating pressure is 20 bar. Since a phase change from liquid to vapour phase occurs, the heat duty is calculated using Equation 29.

**Table 36.** Input data for E-108 heat duty calculation

| Inlet T, °C | Outlet T, °C | n, kmol/s                 | $\Delta H$ at T = 60°C, kJ/kmol | $\Delta H$ at T = -29.12°C, kJ/mol | Calculated Q, kW | Aspen Plus Derived Q, kW |
|-------------|--------------|---------------------------|---------------------------------|------------------------------------|------------------|--------------------------|
| 60          | -29.12       | 0.573241<br>3257606<br>28 | -9094.28                        | -24088.61                          | -8230.38         | -8440.575067<br>296      |

*4.1.8 Heater E-109*

Heater E-109 is used to heat the recycle ethane stream #30 from -8.6°C to 20°C. The operating pressure is 20 bar. Since a phase change from liquid to vapour phase occurs, the heat duty is calculated using Equation 29.

**Table 37.** Input data for E-109 heat duty calculation

| Inlet<br>T, °C | Outlet<br>T, °C | n,<br>kmol/s              | $\Delta H$ at T =<br>-8.6°C,<br>kJ/kmol | $\Delta H$ at T =<br>20°C, kJ/mol | Calculated<br>Q, kW | Aspen Plus<br>Derived Q,<br>kW |
|----------------|-----------------|---------------------------|-----------------------------------------|-----------------------------------|---------------------|--------------------------------|
| -7             | 27              | 0.29961<br>888800<br>4119 | -78874.66                               | -65790.67                         | 3805.68             | 3884.4589423<br>572            |

## 4.2 Water Removal Units

### 4.2.1 Q-101 Quench Tower

The Q-101 unit, located after the E-103 cooler, removes water from the product stream through rapid quenching, preventing polymerization and preparing the gas for downstream processing [63]. Cold water cools the gas from 200°C to 40°C at 4 bar, condensing water and heavy hydrocarbons into wastewater (Stream #10), while the vapor (Stream #11) proceeds to Q-102. The quench water temperature rises from 25°C to 85°C, consistent with industrial practice [64].

The cooling duty, calculated from Aspen Plus enthalpy data, is approximately 17.76 MW. Using

$$Q = mC_p \Delta T \quad (30)$$

the required water flow rate is:

$$m = \frac{Q}{C_p \Delta T} = \frac{17760}{4.18(82-25)} * 3600 = 268345 \text{ kg/hr}$$

This result aligns with industrial data and confirms the feasibility of the design. The design parameters of Q-101 are presented in Table 38.

**Table 38.** Q-101 design specification

| Parameter                    | Value    |                            |                               |
|------------------------------|----------|----------------------------|-------------------------------|
|                              | Inlet    | Stream #10<br>(Wastewater) | Stream #11<br>(Vapor product) |
| Pressure, bar                | 4        | 4                          | 4                             |
| Temperature, °C              | 200      | 40                         | 40                            |
| Vapor fraction               | 1        | 0                          | 1                             |
| Mass flowrate, kg/hr         | 85393.2  | 12388.7                    | 73004.5                       |
| Volume flow, L/min           | 736837   | 210.829                    | 410671                        |
| Enthalpy, J/mol              | -38362.8 | -286512                    | -10447.4                      |
| Total heat duty, kW          | -17760.3 |                            |                               |
| Quench water Temperature, °C | 25       | 82                         |                               |
| Quench water flowrate, kg/hr | 268345   |                            |                               |

#### 4.2.2 Q-102 Dryer

The Q-102 unit removes residual water from the quenched vapor to ensure a fully dry gas before compression. Aspen Plus results show nearly all water is removed into Stream #12, while hydrocarbons remain in Stream #13, with a vapor fraction of 1, confirming complete dehydration.

The heat duty is low (0.34 MW), reflecting minimal thermal effects. This unit prevents condensation in downstream compressors and ensures stable operation.

Zeolite 3A was selected as the adsorbent, with a swing capacity of 7 mmol H<sub>2</sub>O/g (0.13 kg H<sub>2</sub>O/kg adsorbent) [65]. The required adsorbent mass is then calculated based on this capacity.

$$M_{adsorbent} = \frac{m_{water\ removed}}{capacity} \quad (31)$$

**Table 39.** Q-102 design specification

| Parameter                 | Value      |
|---------------------------|------------|
| Operating Temperature, °C | 40         |
| Operating Pressure, bar   | 4          |
| Water in feed, kg/hr      | 1190.27    |
| Water removed, kg/hr      | 1190.15    |
| Heat duty, kW             | -824.184   |
| Adsorbent type            | Zeolite 3A |
| Adsorbent required, kg    | 9155       |

### 4.3 Compressor Units

The production utilizes an array of compressors. To accommodate a reactor operating pressure of 4 bar, a compressor C-101 is positioned upstream to elevate the process pressure from an inlet of 1 bar. This configuration ensures a consistent and regulated gas supply. Compressors C-102, C-103, C-104 are parts of a compressor train, needed for high pressure integrated with a purpose of achieving sufficient pressure for further product separation in columns. C-102 increases pressure from 4 to 10 bars, C-103 increases pressure from 10 to 15 bars and C-104 increases pressure of a stream from 15 to 20 bars. All compressors are operated at 80% efficiency. Values for pressure changes and heat duties are presented in Table 40.

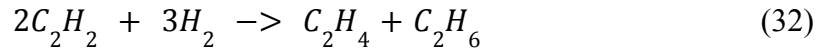
**Table 40.** Compressor units design

|                      | C-101 | C-102 | C-103 | C-104 |
|----------------------|-------|-------|-------|-------|
| Inlet pressure, bar  | 1     | 4     | 10    | 15    |
| Outlet pressure, bar | 4     | 10    | 15    | 20    |
| Heat duty, kW        | 5704  | 2849  | 1643  | 1138  |
| Efficiency           | 0.8   | 0.8   | 0.8   | 0.8   |

### 4.4 Acetylene Removal Unit

During the separation of the components in the distillation columns the problem with the acetylene occurs. Since the boiling points and relative volatilities of acetylene and ethane are very similar, that is why the separation of them is hardly possible. To solve this problem, a new unit was demonstrated to the process - Acetylene Removal Unit. The reactor is placed between the de-ethanizer and C<sub>2</sub> Splitter, so the ethane and ethylene leave the reactor without acetylene.

The reaction that helps to remove this component is called hydrogenation of acetylene with hydrogen to provide the ethane and ethylene as products:



The reaction occurs under 60°C and 20 bar operating conditions [66]. For Aspen simulation, the RStoic reactor type with 100% conversion of acetylene was implemented. Hydrogen content feeded to the reactor is controlled by the Calculator function in Aspen and always supplied at 1.5 times higher than acetylene by the composition. After the reactor, a new cooler is added to the feed for the next separation step. Table 41 shows the operating conditions and heat duty of the acetylene removal unit.

**Table 41.** Acetylene removal unit's design specification.

| Temperature, °C | Pressure, bar | Heat duty, MW |
|-----------------|---------------|---------------|
| 60              | 20            | 1.67          |

## 4.5 Storage Tanks

### 4.5.1 Natural Gas Storage Tank

The natural gas is used as the feed in the ethylene production. The tank should be able to store natural gas for 30 days. The natural gas will be stored at -30 °C on average and 18 bars to ensure liquid phase [67]. Therefore the storage tank will have a smaller volume. The density of the butane at these conditions is taken from Aspen equals to 453.141 kg/m<sup>3</sup>. LPG Sphere Terminal Plant Bulk Tank Farm 10000 m<sup>3</sup> Spherical Tanks have been selected due to the large volume and suitable storage conditions [68].

The required volume was calculated using the equation:

$$V = \frac{Mass}{Density} \quad (33)$$

$$V = \frac{30 \text{ day} * 24 \text{ h/day} * 47438.134 \text{ kg/h}}{453.141 \text{ kg/m}^3} = 75375 \text{ m}^3$$

### 4.5.2 Water Storage Tank

The water is used as feed in the ethylene production. The tank should store water for 30 days. A 10 cubic meter storage facility was selected due to customization [69]. Densities and mass flow rate was taken from Aspen.

The entering feed volume calculated by equation:

$$V = \frac{30 \text{ day} * 24 \text{ h/day} * 13511.46 \text{ kg/h}}{993.957 \text{ kg/m}^3} = 9791 \text{ m}^3$$

The removed water calculated by equation:

$$V = \frac{30 \text{ day} * 24 \text{ h/day} * 13518.67 \text{ kg/h}}{1008.310 \text{ kg/m}^3} = 9653 \text{ m}^3$$

#### 4.5.3 Hydrogen Storage Tank

To optimize storage, hydrogen must be in the liquid stage, but this requires extremely low temperatures. Therefore, it was decided not to store this mixture but to immediately transport it through the pipelines.

#### 4.5.4 Methane Storage Tank

A mixture of gas with a significant amount of methane is a de-methenizer product. For efficient storage, the gas will be cooled to the boiling point of methane, -161 °C. The mixture will be stored in LPG Sphere Terminal Plant Bulk Tank Farm 10000 m<sup>3</sup> Spherical Tanks.

$$V = \frac{30 \text{ day} * 24 \text{ h/day} * 6937.92 \text{ kg/h}}{422.79 \text{ kg/m}^3} = 11815 \text{ m}^3$$

#### 4.5.5 C3+ Storage Tank

The mixture of propane, propylene, and butadiene will be stored under exit conditions from T-104 (20 bar and 88°C). The density of the mixture equals 483.498 kg/m<sup>3</sup>. The mixture will be stored in LPG Sphere Terminal Plant Bulk Tank Farm 10000 m<sup>3</sup> Spherical Tanks.

$$V = \frac{30 \text{ day} * 24 \text{ h/day} * 10238.4 \text{ kg/h}}{484.02 \text{ kg/m}^3} = 15230 \text{ m}^3$$

#### 4.5.6 Ethylene Storage Tank

The ethylene leaves the distillation column at -29.3 °C and 20 bar in vapor phase. For optimal storage, ethylene should be in the liquid form of. For this purpose, ethylene will be stored at a temperature of -30 °C and 20 bar. The required volume of ethylene for 30 days equals to:

$$V = \frac{30 \text{ day} * 24 \text{ h/day} * 27639 \text{ kg/h}}{440.647 \text{ kg/m}^3} = 45161 \text{ m}^3$$

### 4.6 Hydrogen Removal Unit

The hydrogen is removed as a separate stream from other components before the distillation columns tray using the Sep2 model in Aspen with 0.999 split fraction of H<sub>2</sub>. Table 41

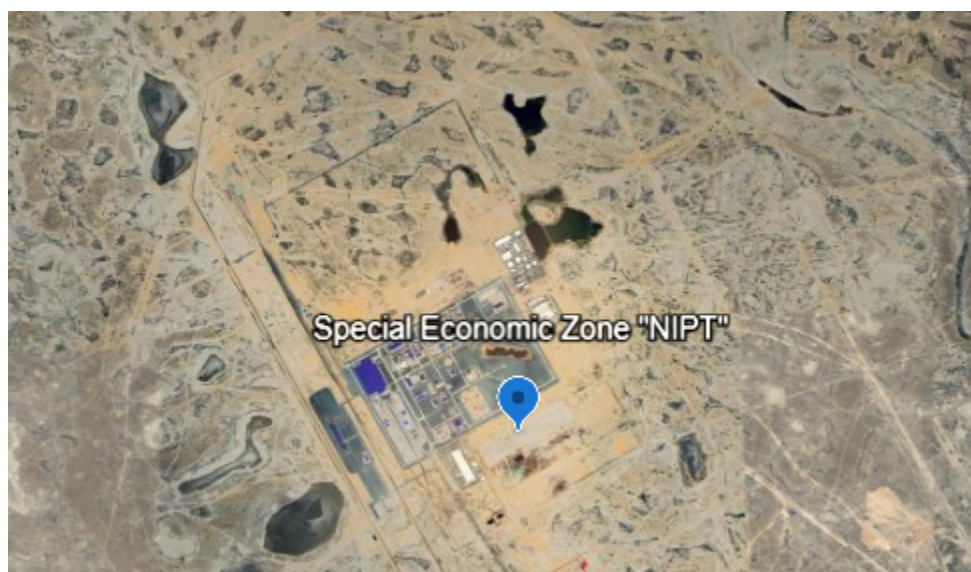
shows the design specification for the separator. Table 42 summarizes the operating conditions and heat duty of the hydrogen removal unit.

**Table 42.** Hydrogen removal unit's design specifications.

| Temperature, °C | Pressure, bar | Heat duty, MW |
|-----------------|---------------|---------------|
| -107.7          | 20            | -0.52         |

## Chapter 5. Plant Location and Layout

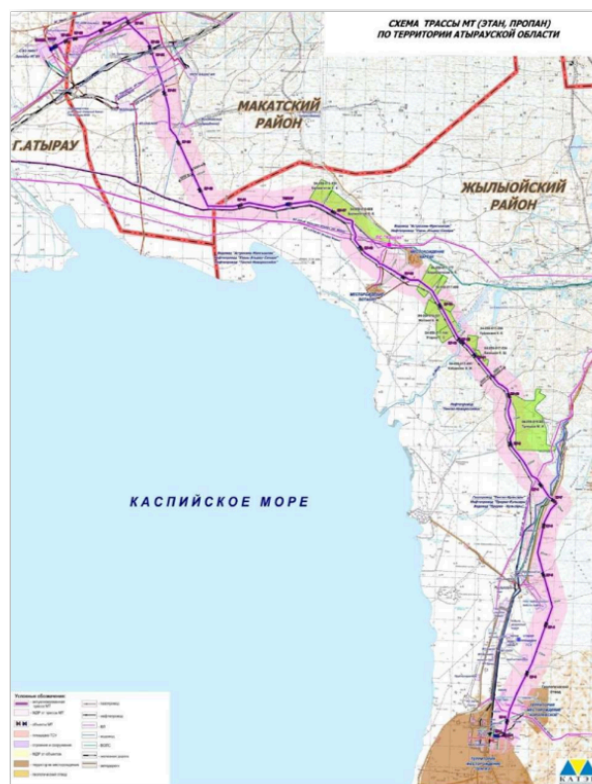
### 5.1 Plant Site Location



**Figure 13.** Karabatan site

Chemical projects require a thorough analysis of possible, suitable locations for the plant. It mainly affects the long-term profitability of the plant, with factors such as feedstock availability, cost of utilities, and logistics being considered as the primary criteria [70]. Primarily, for the ethylene production plant, which requires both high capital investment and continuous access to large volumes of natural gas, the choice of site becomes especially significant. With Tengiz, Kashagan, and Karachaganak located near Atyrau, the region functions as a natural hub for gathering and exporting Kazakhstan's gas. Consequently, the suitable location for an ethylene plant was chosen to be the Atyrau region.

### 5.1.1 Proximity to Raw Materials and Transportation



**Figure 14.** Scheme of the ethane and propane pipeline routes in Atyrau region

Karabatan has a strong strategic advantage because it is located directly along major gas pipeline routes, which makes it an ideal site for petrochemical development within the National Industrial Petrochemical Technopark. This proximity ensures a stable and continuous supply of natural gas as a key feedstock for processes such as ethylene production, while also reducing the need for long-distance transportation and lowering associated costs. Being positioned on existing gas infrastructure improves reliability, minimizes supply risks, and allows faster integration of new industrial projects. In addition, gas distribution systems developed with the involvement of Karabatan Utility Solutions further strengthen the efficiency of resource delivery, making Karabatan a highly attractive and logistically optimized location for large-scale petrochemical plants [71].

### 5.1.2 Infrastructure and Utilities

Building an ethylene plant here has strong advantages due to the well-developed infrastructure of the National Industrial Petrochemical Technopark in Atyrau. The site already has essential transport connections such as roads and railway, along with reliable gas, water and electricity supply systems. A 310 MW power plant and water treatment facilities with a capacity of 15,000 m<sup>3</sup> per day are in operation, ensuring stable utilities for industrial processes. There are

also fire safety systems, pumping stations and logistics areas that support continuous plant operation. Further expansion led by Karabatan Utility Solutions will increase energy capacity and extend water and engineering networks, making the site even more suitable for large scale petrochemical production. This developed infrastructure reduces costs, improves efficiency and allows easy integration with nearby petrochemical projects such as polyethylene and butadiene production [71].

#### *5.1.3 Tax Incentives and Financial Support*

A major advantage of establishing an ethylene plant in Atyrau is its inclusion within the National Industrial Petrochemical Technopark (NIPT SEZ), a Special Economic Zone specifically created to support hydrocarbon processing. Recent reforms to Kazakhstan's SEZ legislation (effective January 2024) introduced a tiered incentive system: large-scale petrochemical projects qualify for extended exemptions from corporate income tax, property tax, land tax, VAT, and customs duties, significantly improving their long-term economic viability [72]. These fiscal incentives reduce operational costs and enhance investor attractiveness, aligning with government strategies to diversify Kazakhstan's economy through petrochemical development.

#### *5.1.4 Climate Considerations*

Atyrau has a sharply continental and semi-arid climate. According to WeatherSpark, In Atyrau, the summers are hot, dry, and mostly clear and the winters are long, freezing, snowy, windy, and partly cloudy. Over the course of the year, the temperature typically varies from -10°C to 33°C and is rarely below -19°C or above 38°C [73]. Overall, the harsh but predictable continental climate of the Atyrau region, combined with its relatively dry conditions, supports safe and reliable plant operation when properly accounted for in design, making it a practical and efficient location from both environmental and operational perspectives.

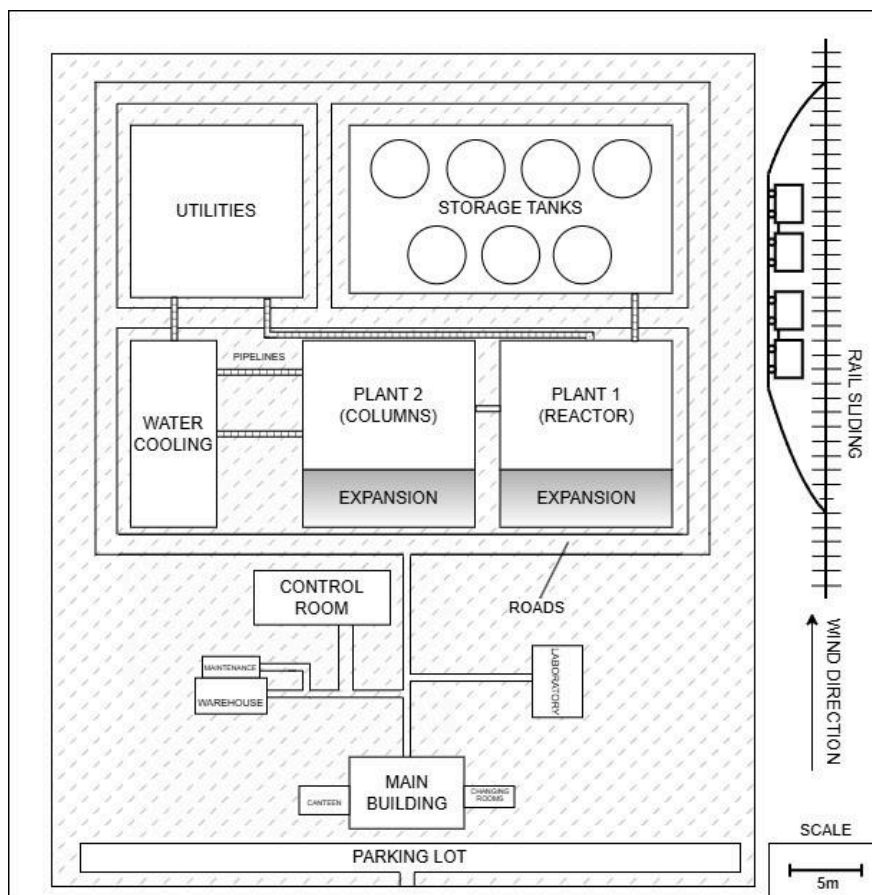
#### *5.1.5 Market Proximity*

Locating the plant close to the emerging Silleno project as a main buyer provides a major strategic advantage, as it ensures stable demand and reduces transportation costs. Short distances between producer and consumer improve supply reliability, lower logistical risks, and allow more efficient integration within the petrochemical value chain, making operations more cost-effective and competitive [73].

### *5.2 Plant Layout*

The ethylene production plant layout was designed to ensure safe operation, efficient process flow, and easy maintenance, and can be seen on Figure 15. The site is divided into six main areas: Reactor, Columns, Utilities, Storage, Administrative, and Water Cooling. Each section is planned according to the process steps and safety requirements. The Reactor area

houses the main ethylene reactor, where the primary reaction occurs, while the Columns area includes the distillation columns, which are essential for separating and purifying the product. The Utilities area provides the necessary infrastructure for power, gas, and other utilities required for operation. The Storage area is dedicated to the storage tanks and equipment related to the safe storage of materials, and the Administrative area contains the main building, which includes offices, laboratories, and other support functions, which are located in a safe distance from the plant area and moved, upwind of it, in case of any leak emergencies. Lastly, the Water Cooling section is responsible for maintaining the cooling system necessary for safe plant operation. This layout ensures a streamlined process, while prioritizing safety and accessibility for all operations and support activities. The whole plant requires 284200m<sup>2</sup> of space with dimensions of 490m to 580m.



**Figure 15.** Suggested plant layout

### 5.2.1 Production and Utility

The main production units are strategically located in the heart of the plant, forming the operational core. This area includes the ethylene reactor, where the primary reaction takes place, supported by distillation columns for product separation and purification. Additionally, heat exchangers are integrated into this section to manage thermal energy within the system. Surrounding the central reaction area are auxiliary units like furnaces, a three-phase separator,

and other heat integration systems that play critical roles in maintaining process control. Utility systems such as steam generation, cooling water, and power distribution are situated nearby, ensuring that the production process runs smoothly without interruptions or pressure drops. Fire safety stations are strategically placed on both sides of the plant to ensure full coverage, complying with industrial safety standards and enabling rapid emergency response. The layout also ensures adequate space for maintenance access, provides safe distances between hazardous units, and facilitates efficient vehicle movement when necessary.

### *5.2.2 Storage, Monitoring, and Waste Management*

The storage area is located adjacent to, but clearly separated from, the process units, with careful attention given to safety and environmental considerations. It includes dedicated tanks for raw materials such as natural gas and water, product storage tanks for ethylene and hydrogen, and waste holding facilities including the wastewater storage tank. Additional tanks for methane and  $C_3^+$  byproducts are also positioned within this zone. Each tank is placed with fire safety and spill prevention as primary considerations. Close to the production area, the control room and quality laboratory are situated. The control room oversees the entire plant through automated monitoring systems, alarms, and sensors, while the laboratory handles quality verification and compositional analysis of process streams throughout operation. A first aid station is placed within this zone to enable rapid response to any incidents.

### *5.2.3 Administrative and Support Zone*

All non-process and personnel-related facilities are grouped together and positioned at a safe distance from the main process area. This zone includes an administrative building housing engineering and management offices, as well as support structures providing accommodation and welfare facilities for operational and technical staff. Adjacent to these buildings, canteen and warehouse facilities ensure that workers have access to meals and essential supplies without needing to leave the plant site. The plant is served by a dedicated internal road network that facilitates the movement of materials, personnel, and emergency vehicles. Heavy vehicle routes are segregated from pedestrian pathways to maintain safety throughout the site.

## **Chapter 6. Process Safety and Environment Management**

This chapter addresses the key safety, health aspects and environment management of the main process components, including methane, ethane, ethylene, propane, hydrogen, propylene, acetylene, butadiene, and hydrogen with a summary of their associated hazards. Detailed NFPA hazard classification tables for these substances are provided in the Appendix F.

### 6.1 HAZOP Analysis of Major Units

HAZOP analysis is conducted for each major equipment to study the risk that can appear from each unit. Table 43-46 shows the hazards for units.

**Table 43.** HAZOP analysis for H-101 Reactor.

| Item | Parameter   | Guide word | Deviation                               | Possible causes                            | Consequences                                                            | Action required                                                      |
|------|-------------|------------|-----------------------------------------|--------------------------------------------|-------------------------------------------------------------------------|----------------------------------------------------------------------|
| 1A   | Flow        | No         | Cooling coils fails                     | Control valve fails closed                 | Loss of cooling, possible runaway.                                      | 1. Select valve to fail open.                                        |
|      |             |            |                                         | Plugged cooling coils                      |                                                                         | 2. Install filters with maintenance procedure.                       |
|      |             |            |                                         | Cooling water service failure.             |                                                                         | Install cooling water flow meter and low-flow alarm.                 |
|      |             |            |                                         | The controller fails and closes the valve. |                                                                         | Install high temperature alarm to alert operators.                   |
|      |             |            |                                         | Air pressure fails, closing valve.         |                                                                         |                                                                      |
| 1B   | Flow        | More       | Cooling coils fails                     | Control valve fails closed                 | Reactor cools, reactor concentration builds, possible sleeping reactor. | 1. Instruct operators and update procedures.                         |
|      |             |            |                                         | The controller fails and opens the valve.  |                                                                         | 1. Place controller on critical instrumentation list.                |
|      |             |            |                                         |                                            |                                                                         |                                                                      |
| 1C   | Flow        | Less       | Cooling coils fails                     | Partially plugged cooling coils.           | Diminished cooling, possible runaway.                                   | 1. See 1A.2                                                          |
|      |             |            |                                         | Partial water source failure.              |                                                                         | 2. Place valve on critical instrumentation list.                     |
|      |             |            |                                         | The control valve fails to respond.        |                                                                         |                                                                      |
| 2A   | Temperature | More       | Temperature of the fuel gas is too high | Temperature indicator controller failure   | Failure to achieve desired yield                                        | Install high temperature alarm                                       |
|      |             |            |                                         | Wrong set point at temperature controller  | Secondary reactions occur                                               | Operator should insure the temperature sensor is in a good condition |

| Item | Parameter | Guide word | Deviation                                      | Possible causes                                                                           | Consequences                                                                                                                                                                                | Action required                                                                 |
|------|-----------|------------|------------------------------------------------|-------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------|
| 2B   |           | Less       | Temperature in the reactor is low              | Temperature indicator controller malfunctions<br><br>Control valve for steam failure      | No reaction occur<br><br>Failed to produce a huge volume of cracked effluent gas in a short time                                                                                            | Install low temperature alarm                                                   |
| 3A   | Pressure  | More       | Pressure of coil inlet is too high from normal | Pressure indicator controller malfunctions<br><br>Level indicator controller malfunctions | Possible overheating due to high pressure<br><br>Frequent leaking                                                                                                                           | Install high pressure alarm<br><br>Adjust the setting on pressure control valve |
| 3B   |           | Less       | Pressure of the fuel gas is too low            | Failure at the fuel gas header or upstream refinery gas supply.                           | When serious, it may lead to flameout. If there is a fuel gas pressure fluctuation, the furnace is in danger of a secondary flash explosion.<br><br>Incomplete combustion and CO formation. | Low-pressure alarm, pressure control loops.                                     |

**Table 44.** HAZOP analysis for E-105 Cooler [74].

| Item | Parameter          | Guide word | Deviation        | Possible causes                      | Consequences                        | Action required                          |
|------|--------------------|------------|------------------|--------------------------------------|-------------------------------------|------------------------------------------|
| 1A   | Flow               | More       | High flow        | Excessive coolant flow               | Inefficient cooling, energy waste   | Install flow restrictors in coolant line |
| 2A   | Temperature        | More       | High temperature | Malfunction of temperature control   | Overheating of heat exchanger tubes | Install backup temperature sensors       |
| 3A   | Pressure           | Less       | Low pressure     | Loss of pressure control             | Potential for vapor lock in system  | Use dual pressure regulators             |
| 4A   | Emergency shutdown | Reverse    | No reaction      | Failure of emergency shutdown system | Delayed response to hazards         | Conduct regular tests of shutdown system |

**Table 45.** HAZOP analysis for E-110 Heater [75, 76].

| Item | Parameter     | Guide word    | Deviation                           | Possible causes                             | Consequences                                   | Action required                                        |
|------|---------------|---------------|-------------------------------------|---------------------------------------------|------------------------------------------------|--------------------------------------------------------|
| 1A   | Flow          | No            | No flow                             | Pump failure, valve closed                  | Overheating, local hot spots                   | Add trip on no flow or temperature deviation           |
| 1B   | Flow          | Less          | Low flow                            | Fouling, partial blockage, valve throttling | Insufficient heating, reactor feed issues      | Routing cleaning and inspections                       |
| 2A   | Temperature   | Less          | Low temperature                     | Heater underperformance                     | Incomplete reactions in the process            | Install low temperature alarm or secondary heat source |
| 3A   | Pressure      | More          | More pressure in tube side          | Failure of process fluid valve              | Bursting of tube                               | Install high pressure alarm                            |
| 4A   | Fluid quality | Contamination | Contamination of process fluid line | Leakage of tube and water goes in           | Contamination of process fluid and composition | Proper maintenance and operator alert                  |
| 5A   | Corrosion     | Corrosion     | Corrosion of tube                   | Hardness of cooling water                   | Less cooling and crack of tube                 | Proper maintenance                                     |

**Table 46.** HAZOP analysis for T-101/T-102/T-103 [77-80].

| Item | Parameter | Guide word | Deviation | Possible causes             | Consequences                                                                                           | Action required                                                                       |
|------|-----------|------------|-----------|-----------------------------|--------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|
| 1A   | Flow      | No / None  | No flow   | No flow of feed to column   | Pipe blockage; pump failure; feed valve closed; upstream equipment shutdown                            | Column dry-out; product off-specification; potential damage to reboiler; loss of feed |
| 1B   | Flow      | More       | High flow | High flow of feed to column | Feed control valve failure (open); upstream pressure surge; operator error                             | Column flooding; poor separation; off-spec overhead product; increased condenser load |
| 1C   | Flow      | Less       | Low flow  | Low reflux flow             | Reflux pump failure; partial pipe blockage; reflux control valve malfunction; low level in reflux drum | Reduced separation; high content in bottom product; reduced ethylene recovery         |

| Item | Parameter   | Guide word | Deviation        | Possible causes                       | Consequences                                                                                                     | Action required                                                                                                   |
|------|-------------|------------|------------------|---------------------------------------|------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| 2A   | Pressure    | More       | High pressure    | High pressure in column               | Condenser cooling water failure; overhead valve failure (closed); non-condensable gas accumulation; blocked vent | Column overpressure; risk of rupture or PSV activation; flammable gas release; equipment damage                   |
| 2B   | Pressure    | Less       | Low pressure     | Low pressure in column                | Large leak; overhead valve failure (open); sudden feed temperature drop; loss of reboiler duty                   | Possible air ingress; change in relative volatility; poor separation; risk of two-phase flow; off-spec products   |
| 3A   | Temperature | More       | High temperature | High temperature in column / reboiler | Excess reboiler steam supply; reboiler control valve failure; loss of overhead cooling; wrong feed composition   | Thermal degradation; excess vaporisation; losses in bottom product; possible overpressure; poor ethylene recovery |
| 3B   | Temperature | Less       | Low temperature  | Low temperature in column             | Insufficient reboiler duty; steam supply failure; excessive cold feed; loss of heat tracing                      | Inadequate separation; high product in bottom (C <sub>2</sub> +); risk of freezing/hydrate formation.             |

## 6.2 Process Waste Streams

During the design and construction phases of industrial plants, it is essential to carefully evaluate potential emissions, waste streams, and the broader environmental impacts associated with the production processes.

There are 4 waste streams in the entire process system - top product of T-100 separator, top product of T-101 column, bottom product of T-102 product, and wastewater stream after quench tower and dryer. Compositions and mass flow rates of these streams shown in Table 47.

**Table 47.** Mass flow rate of wastestreams.

| Compound  | Mass flow rate, kg/hr |                         |                   |
|-----------|-----------------------|-------------------------|-------------------|
|           | Top product of T-101  | Bottom product of T-102 | Wastewater stream |
| Methane   | 6816.5                | 0                       | 0.68943           |
| Propane   | 0                     | 1318.8                  | 0.13232           |
| Ethylene  | 127.99                | 0                       | 3.3491            |
| Propylene | 0                     | 583.90                  | 0.088670          |
| Hydrogen  | 2.6560                | 0                       | 0.26610           |
| Ethane    | 0.10764               | 0                       | 2.6489            |
| Water     | 0                     | 0.11984                 | 13511             |
| Acetylene | 0.19009               | 0                       | 0.038249          |
| Butadiene | 0                     | 8339.4                  | 0.83626           |
| Total     | 6947.4                | 10242                   | 13519             |

### 6.2.1 Wastewater Stream

This stream consists mainly from water, wt% 99.9%, which can be purified for further reuse in the production process. However, the stream contains some amount of light organic compounds such as Ethylene (wt% 0.025%), and ethane (wt% 0.02%). Reverse osmosis (RO) membrane systems are among the most efficient and economical methods for purification. They can effectively remove and concentrate trace organic contaminants enabling the production of clean water that can be reused or safely discharged. This approach helps conserve freshwater resources, reduces environmental impact, and decreases overall treatment expenses [81].

### 6.2.2 Top Product of T-101 Column

The top product of the T-101 demethanizer column consists predominantly of methane (approximately 98.0 wt%), with minor amounts of ethylene (wt% 1.99%) and trace quantities of ethane and acetylene. This waste stream can be utilized as a fuel source within the primary production process. All organic components present in this stream carry considerable fuel value, as reflected in its high gross heating value. Combustion of this methane-rich stream can supply thermal energy to the H-101 fired furnace, partially offsetting the external fuel gas demand and improving the overall energy efficiency of the plant.

### 6.2.3 Bottom Product of T-102 Column

This waste stream can be utilized as a fuel source in the primary production processes, as it does not contain flammable light organic gases or hydrogen. Additionally, recovering materials from this stream is not economically viable, especially when considering the significant investment required for distillation columns. All the organic components in this stream have considerable fuel value, as indicated by the total stream's gross heating value of about 47517.45

kJ/kg. The water content in this stream is minimal, allowing it to be burned directly to provide energy for the main production process. Due to its high combustion energy, the stream can also be split into multiple portions to supply energy to different units within the system.

### *6.3 Emission Control Systems*

Ethylene production involves intensive chemical processes that release substantial quantities of carbon dioxide, nitrogen oxides, and volatile organic compounds. Managing these effluents is critical for maintaining regulatory compliance and reducing the overall environmental burden of the facility [82].

Effective emission control starts with accurate detection of pollutants. Technologies such as continuous emission monitoring systems (CEMS) are essential for real-time tracking of pollutants like greenhouse gases, nitrogen oxides, and volatile organic compounds (VOCs). These systems typically use sensors to measure gas concentrations in flue gases and other process emissions, providing data that helps operators adjust processes to minimize emissions. For CO<sub>2</sub> detection, infrared absorption sensors are commonly used, as they can precisely measure gas concentrations at various stages of production. Similarly, nitrogen oxides detection often relies on chemiluminescence analyzers, which react with nitrogen oxides to emit light, directly correlating to their concentration. VOCs are frequently monitored using flame ionization detectors (FID), which measure the ionization of carbon atoms in VOC molecules when exposed to a flame. By integrating these detection systems, the plant can ensure that emissions remain within legal limits and can promptly address any unexpected increases in pollutant levels [82].

The primary release of carbon dioxide occurs during hydrocarbon combustion in the H-101 fired furnace and through waste streams. In the combustion process of the waste streams, a significant amount of carbon dioxide will be released into the environment. The total yearly carbon dioxide generated by this stream was calculated in Aspen Plus using an RGibbs reactor, under the assumption of 100% conversion of all hydrocarbons and aromatics into combustion products. The total rate of greenhouse gas production from combustion of the waste stream is 32,920 kg/hr, which corresponds to approximately 288,379 tons/year of greenhouse gas emissions. In addition, the utility-related CO<sub>2</sub> emissions calculated in Aspen Plus amount to 21,759 kg/hr, corresponding to approximately 190,569 tons/year. The combined total greenhouse gas emissions from both sources are therefore approximately 478,948 tons/year. To mitigate these levels, the plant can adopt carbon capture and storage to sequester emissions underground or carbon capture utilization to transform the gas into secondary products like methanol or biofuels [82, 83]. Furthermore, transitioning to low-carbon fuel sources and integrating renewable energy into the grid can lower the total carbon footprint of the operation [83].

Nitrogen oxides are generated as a byproduct of the combustion process. Control is achieved through the implementation of low-nitrogen oxide burners, which suppress the formation of

these compounds by regulating flame temperature and the mixing of air and fuel. For post-combustion treatment, selective catalytic reduction or selective non-catalytic reduction technologies are utilized to convert nitrogen oxides into harmless nitrogen and water vapor, ensuring the facility meets air quality standards [84].

Volatile organic compounds are typically emitted from process vents and storage facilities. These emissions are managed through thermal or catalytic oxidation, processes that decompose the organic compounds into carbon dioxide and water at high temperatures. Additionally, the use of vapor recovery units and floating roof designs on storage tanks serves to capture fugitive emissions, preventing their release into the atmosphere and improving overall resource efficiency [82].

The ethylene production plant in the Atyrau region is governed primarily by the Environmental Code of the Republic of Kazakhstan (No. 400-VI, 2021) [85]. Under Article 111, an integrated environmental permit is mandatory for Category I installations, and under Article 186, operators must monitor and report emissions to the government, with Category I facilities required to maintain an automated real-time emissions monitoring system.

## **Chapter 7. Total Investment and Profitability**

This chapter will observe the total investments and overall profitability of the ethylene production plant, providing economic analysis of factors such as prices of raw materials and final product, costs of equipment, fixed costs, and variable costs. The manual economic calculations will be presented using Aspen Process Economic Analyzer (APEA) and Capital Cost Estimation tool (Capcost). The extensive calculations can be found in ESI Escel file.

### *7.1 Price of Raw Materials and Final Product*

Before starting the economic analysis of the plant, it is important to evaluate the cost of natural gas as one of the key raw materials. It should be noted that natural gas prices are strongly influenced by global crude oil and gas market trends, as well as regional supply–demand dynamics. By conducting a comparative analysis of natural gas prices across different countries and regions, as presented in Table 48 below, it can be observed that significant price variations exist. Among the considered options, Kazakhstan offers relatively low natural gas prices (2.94 USD/MMBtu), comparable to those in the USA (2.85 USD/MMBtu) and lower than in regions such as Europe (13.51 USD/MMBtu) and the Asia-Pacific (10.75 USD/MMBtu). Therefore, sourcing natural gas locally from Kazakhstan is considered the most economically feasible option for the plant.

**Table 48.** Global prices of raw materials

| Seller country or region | Price of natural gas, USD/MMBtu |
|--------------------------|---------------------------------|
| USA                      | 2.85 [86]                       |
| China                    | 1.93 [87]                       |
| Saudi Arabia             | 2.44 [87]                       |
| Asia-Pacific region      | 10.75 [88]                      |
| Kazakhstan               | 2.94 [89]                       |
| Europe                   | 13.51 [87]                      |

It is also important to take into account the selling price of natural gas. In this case, global ethylene prices in 2026 were analyzed and are presented in Table 49.

**Table 49.** Global prices of final products

| Ethylene [90]  |       |                  |        |                |                |
|----------------|-------|------------------|--------|----------------|----------------|
| Region         | Japan | Northwest Europe | China  | Southeast Asia | Northeast Asia |
| Price, USD/ton | 1475  | 1567             | 1350.0 | 1475           | 1425           |
| Hydrogen [91]  |       |                  |        |                |                |
| Region         | USA   | Saudi Arabia     | UAE    | Japan          | Netherlands    |
| Price, USD/ton | 1096  | 2161             | 2941   | 2500           | 2275           |

By analyzing the prices of the main products, approximate selling prices of the target products can be estimated. As shown in Table 48, ethylene prices are generally lower in Asian regions such as China and Southeast Asia compared to Europe. Based on this trend, the preliminary predicted price for ethylene is assumed to be 1,450 USD per tonne.

Similarly, hydrogen prices exhibit noticeable regional variation, with lower prices observed in the USA and relatively higher prices in regions such as the Netherlands and Japan. Taking this into account, the preliminary predicted price for hydrogen is estimated at 2,200 USD per tonne.

## 7.2 Cost of Equipment and Storage Tanks

The cost of equipment for plant operation was estimated using APEA and Capcost 2017. After determining the equipment costs, the values obtained from APEA were adjusted by applying their respective Lang factors [92] and a location factor of 1.32. The location factors accounted to the distance between China and Atyrau. Cost escalation was calculated using the CEPCI factors from the reference book (532.9) and the projected value for March 2026 (830). The total cost of equipment was calculated to be roughly 284,878,500 USD. The results are shown in Table 50.

**Table 50.** Equipment cost

| Type                 | Name  | Equipment cost | Installed cost | Location factor | Lang factor*CEPCI |
|----------------------|-------|----------------|----------------|-----------------|-------------------|
| Compressors          | C-101 | \$3,363,611    | \$3,363,611    | \$5,146,325     | \$20,038,701      |
|                      | C-102 | \$3,952,800    | \$4,365,200    | \$6,678,756     | \$26,005,665      |
|                      | C-103 | \$1,557,400    | \$1,876,800    | \$2,871,504     | \$11,181,030      |
|                      | C-104 | \$1,374,300    | \$1,682,800    | \$2,574,684     | \$10,025,275      |
| Heaters              | E-101 | \$32,200       | \$137,700      | \$210,681       | \$1,148,486       |
|                      | E-102 | \$38,100       | \$167,400      | \$256,122       | \$1,396,199       |
|                      | E-103 | \$4,950,000    | \$10,500,000   | \$16,065,000    | \$25,021,486      |
|                      | E-109 | \$20,500       | \$108,600      | \$166,158       | \$258,794         |
|                      | E-110 | \$22,300       | \$109,100      | \$166,923       | \$909,948         |
| Coolers              | E-104 | \$3,760,000    | \$5,873,000    | \$8,985,690     | \$13,995,351      |
|                      | E-105 | \$41,300       | \$162,100      | \$248,013       | \$386,284         |
|                      | E-106 | \$41,400       | \$162,000      | \$247,860       | \$1,351,160       |
|                      | E-107 | \$466,900      | \$790,700      | \$1,209,771     | \$6,594,830       |
|                      | E-108 | \$278,200      | \$504,300      | \$771,579       | \$4,206,112       |
| Reactors             | H-101 | \$6,660,000    | \$8,080,000    | \$12,362,400    | \$19,254,629      |
|                      | H-102 | \$23,000       | \$92,200       | \$141,066       | \$282,132         |
| Quench Tower         | Q-101 | \$69,400       | \$293,700      | \$449,361       | \$1,797,444       |
| Dryer                | Q-102 | \$53,300       | \$241,200      | \$369,036       | \$1,476,144       |
| Distillation Columns | T-100 | \$88,300       | \$352,300      | \$539,019       | \$3,358,122       |
|                      | T-101 | \$722,900      | \$1,995,900    | \$3,053,727     | \$19,024,908      |
|                      | T-102 | \$1,739,300    | \$2,810,300    | \$4,299,759     | \$26,787,765      |
|                      | T-103 | \$5,529,900    | \$8,287,400    | \$12,679,722    | \$78,995,453      |
| Storage Tanks        |       |                |                | \$11,382,581    |                   |
| Total cost           |       |                |                | \$90,875,737    | \$284,878,500     |

The cost of the storage units was estimated based on the weight of each tank and the unit price of the material used. For stainless steel (SS316), the unit price was taken as 2.52 USD/kg

[93], while fiberglass was priced at 1.8 USD/kg [94]. The total cost required for the storage tanks was calculated to be approximately 11,382,581 USD. The detailed cost estimates are presented in Table 51.

**Table 51.** Storage tanks cost estimation

| ID            | TK-101     | TK-102      | TK-103      | TK-104      | TK-105      | TK-106      | TK-107     |
|---------------|------------|-------------|-------------|-------------|-------------|-------------|------------|
| Component     | Water      | Natural gas | Methane     | Ethylene    | C3+         | Hydrogen    | Wastewater |
| Material      | Fiberglass | SS316       | SS316       | SS316       | SS316       | SS316       | Fiberglass |
| Price, USD/kg | 1.8        | 4.951       | 4.951       | 4.951       | 4.951       | 4.951       | 1.8        |
| Price, USD    | \$48,960   | \$2,766,357 | \$1,039,537 | \$2,850,266 | \$1,558,851 | \$1,893,128 | \$59,106   |

### *7.3 Total Fixed Capital Cost Investment Estimation*

To estimate the total capital investment, it is necessary to evaluate the Inside Battery Limit (ISBL), Outside Battery Limit (OSBL), engineering costs, and contingency charges. ISBL includes the costs of equipment, installation, construction, and other expenses that directly reflect the cost of the plant.

The ISBL cost was taken directly from the total equipment cost, which was estimated to be USD 284,878,500. The ISBL represents the cost of the main process units and associated plant items installed within the battery limits.

OSBL refers to the offsite expenditures required for additional infrastructure and supporting facilities outside the main plant battery limits. In most cases, these costs are estimated as approximately 40% of the ISBL. Based on this assumption, the OSBL cost was calculated to be approximately USD 113,951,400.

Engineering Costs (EC), which include detailed design, engineering services, procurement support, and project management activities, were calculated as 30% of the combined ISBL and OSBL costs. This gives an estimated Engineering Cost of approximately USD 119,648,970.

Contingency charges, which account for potential cost variations such as market fluctuations and uncertainties during project implementation, were assumed to be 10% of the total ISBL and OSBL cost. Accordingly, the Contingency cost was estimated at approximately USD 39,882,990.

The summary of the capital investment estimation is presented in the Table 52.

**Table 52.** Estimations of capital investment

| Capital cost component | Cost, USD          |
|------------------------|--------------------|
| ISLB                   | 284,878,500        |
| OSLB                   | 113,951,400        |
| Engineering cost       | 119,648,970        |
| Contingency cost       | 39,882,990         |
| <b>Total</b>           | <b>558,361,860</b> |

#### 7.4 Fixed and Operating Labor Costs

Fixed and operating labor costs were estimated based on the number of major equipment units in the plant and the requirement for continuous operation. Since the plant is designed for 24-hour industrial production, labor requirements were determined for shift operators as well as additional personnel involved in maintenance and plant support activities.

##### 7.4.1 Operating Labor Cost Estimation

The number of operating personnel was estimated based on the number of major process units requiring continuous monitoring, including compressors, heat exchangers, reactors, separation units, and storage facilities. The estimates were based on the correlation proposed by Alkhayat and Gerrard [95]:

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5} \quad (34)$$

Where,  $N_{OL}$  is the number of operating labour workers,  $P$  is the process steps handling solids,,  $N_{np}$  is the number of process steps not involving handling solids.

The total number of equipment  $N_{np}$  is 29, excluding auxiliary components such as valves and mixers, since they do not require dedicated operating personnel.  $P$  is taken as 0 as no solids are involved in the process. Thus,  $N_{OL}$  is equal to 3.6, meaning approximately 4 operators are required per shift. Taking an ideal operation of plant (365 days a year), resulting in  $Y$  number of shifts per year. A single operator works about 49 weeks a year, 5 days a week (8 hours), meaning 245 shifts per year. Finally, 18 number of operators is needed.

The operating labor can be calculated as follows:

$$\text{Operating labor} = N_{OL} * N_{np} \quad (35)$$

The cost of operating labor is calculated using:

$$C_{OL} = \text{Operating Labor} * \text{Average Salary} \quad (36)$$

For continuous 24-hour operation, 18 operators per shift were assumed. Considering multiple shifts and additional staffing requirements, the total number of operators was estimated as 72. Using an average annual salary of 7,583 USD per operator, the direct operating wages and benefits were estimated as 545,953 USD/year.

**Table 53.** Labor cost estimation parameters

| Parameter                   | Value     |
|-----------------------------|-----------|
| Number of equipment units   | 29        |
| Operators per shift         | 18        |
| Overall number of operators | 72        |
| Average salary per operator | \$7,583   |
| Direct wages and benefits   | \$545,953 |

#### 7.4.2 Fixed Costs Estimation

In addition to direct operating wages, total labor-related operating costs include salaries and benefits for supervisory and supporting personnel, operating supplies and services, technical assistance to manufacturing, and control laboratory expenses. These costs were estimated using standard cost-estimation factors and spreadsheet-based calculations. As a result, the total labor-related operating cost was estimated as 1,479,5338 USD/year.

The operating costs of the plant include essential overheads for maintenance, operations, and services. Maintenance-related costs were also considered separately, including wages and benefits, materials and services, and maintenance overhead. These costs are important due to the large number of equipment units and the need for reliable operation of compressors, heaters, reactors, and separation columns. The total maintenance cost was estimated as 4,674,164 USD/year. The total operating overhead amounts to 6,410,303 USD/year, which covers areas such as maintenance and operations (5,220,117 USD), plant overhead (370,628 USD), mechanical services (125,283 USD), human resource department and business services (694,276 USD). Additionally, the general plant overhead is estimated at 10,410,206 USD/year.

Other fixed costs, including property tax and insurance (1,555,290 USD) and environmental charges (1,451,604 USD), are based on the plant's investment cost (1.5% of ISBL, and 1% of ISBL+OSBL respectively). The total fixed costs of production, including equipment, amount to 19,570,796 USD/year, with the combined total cost for fixed production and equipment estimated at 246,360,897 USD.

## 7.5 Variable Cost of Production

Variable cost of production includes all expenses that change with production rate. For this plant, the major variable cost components are raw materials, utilities, and waste treatment.

### 7.5.1 Cost of Raw Materials

The cost of raw materials was estimated using the mass flow rates obtained from Aspen simulation and the corresponding market prices of the main process streams. Annual raw material costs were calculated by multiplying the feed flow rate of each component by its unit price and the yearly operating time. Since raw materials directly determine the production capacity, this cost represents a major contribution to the variable operating costs of the plant.

Natural gas, used as fuel, is priced at 2.94 USD/MMBtu, which contributes 2,693 USD/year for its consumption in stream 1. Water, a major raw material, is priced at 0.78 USD per liter [96], with a total annual cost of 92,882,392 USD/year for stream 3. In terms of products, hydrogen is valued at 2,200 USD/tonne, resulting in a total value of 51,134,413 USD/year. Ethylene, produced in stream 31-1, is valued at 1,450 USD/tonne, contributing 350,902,449 USD/year to the total product revenue. The total cost for raw materials is 92,885,086 USD/year, while the total product revenue amounts to 402,036,862 USD/year. Detailed calculations and assumptions used in determining the annual raw material costs are provided in the ESI.

**Table 54.** Estimation of raw materials

| Raw Material | Stream | Price         | Annual Cost, \$/y |
|--------------|--------|---------------|-------------------|
| Natural gas  | 1      | 2.94 \$/MMBtu | 2,693             |
| Water        | 3      | 0.78 \$/L     | 92,882,392        |
| Hydrogen     | 23     | 2200 \$/tonne | 51,134,413        |
| Ethylene     | 31-1   | 1450 \$/tonne | 350,902,449       |

### 7.5.2 Cost of Utilities

Utility costs were estimated based on the energy requirements obtained from process simulation and corresponding unit prices. The main utilities identified include electricity, cooling water, refrigerants, and steam used in various process units. The total utility consumption was converted into annual costs based on continuous plant operation. The total cost of utilities was calculated to be 22,501,544 USD/year.

### *7.5.3 Cost of Waste Treatment*

To evaluate the cost of waste treatment, it is essential to identify the process streams that require purification before discharge or reuse. In the present process, the primary stream requiring treatment is the wastewater stream generated after the quench tower, as other byproduct streams are utilized as fuel within the plant. This wastewater stream consists predominantly of water (approximately 99.9 wt%), with minor amounts of light organic compounds such as ethylene and ethane.

The treatment of this stream is proposed to be carried out using reverse osmosis (RO) membrane systems, which are effective in removing dissolved contaminants and enabling water reuse within the process. Based on the process simulation, the mass flow rate of the wastewater stream is 13,511 kg/h. Assuming a density equivalent to water, this corresponds to a volumetric flowrate of approximately 13.51 m<sup>3</sup>/h. For continuous plant operation at 8760 hours per year, the annual wastewater volume is estimated to be 118,359 m<sup>3</sup>/year.

To estimate the cost of wastewater treatment, a representative treatment cost of 3.63 USD/m<sup>3</sup> was adopted [97]. Therefore, the annual operating cost of wastewater treatment is calculated to be 429,644 USD/year. In addition, the installed cost of the wastewater treatment unit is estimated at 31,593 USD. When annualized over a 20-year equipment lifetime, this corresponds to an additional cost of 1,580 USD/year. Consequently, the total annual cost associated with wastewater treatment is estimated to be 431,224 USD/year.

## *7.6 Economic Analysis*

### *7.6.1 Revenue Estimation*

The total revenue of the plant is derived from the sale of ethylene, hydrogen, methane, and C<sub>3</sub><sup>+</sup> gas. Product prices were assigned based on regional market analysis, with ethylene priced at 1450 USD/tonne and hydrogen at 2200 USD/tonne. These values were implemented in Aspen Plus, where product flow rates were used to calculate the corresponding revenue contributions for each stream.

The total revenue from Hydrogen, priced at \$2200 per tonne, amounts to \$51,134,413 from Stream 23. On the other hand, the total revenue from Ethylene, priced at \$1450 per tonne, contributes \$350,902,449 from Stream 31-1. Combining these values, the total revenue from both products equals \$402,036,862. This breakdown shows that ethylene generates the bulk of the revenue, contributing around 87.3% of the total, while hydrogen contributes approximately 12.7%.

**Table 55.** Ethylene plant revenue by product

| Product  | Revenue       |
|----------|---------------|
| Ethylene | \$51,134,413  |
| Hydrogen | \$350,902,449 |
| Total    | \$402,036,862 |

### 7.6.2 Expenses Estimation

The total capital investment for the plant is estimated to be USD 558,361,860. The annual operating expenses are categorized into fixed and variable costs. The total fixed cost of production is approximately USD 48,333,340 per year, which includes labor costs (USD 545,953/year), maintenance expenses (USD 12,842,323/year), and operating overhead (USD 16,440,803/year). Additionally, there are charges for property tax and insurance (USD 4,273,178), as well as environmental charges (USD 3,988,999), which are calculated as 1.5% of ISBL + OSBL.

The annual variable cost of production is approximately USD 115,817,854, with utilities contributing USD 22,501,544 and raw materials (such as natural gas and water) accounting for USD 92,885,086. The costs associated with wastewater treatment are calculated at USD 431,224 per year.

Moreover, the plant is subject to a corporate income tax of 20% on the total capital investment. This tax will be applied at the end of the first year, reflecting potential variations in production capacity, market conditions, and inflation. The detailed breakdown of these production-related expenses is summarized in Table 56.

**Table 56.** Major ethylene production expenses

| Expenses                                                | Value       |
|---------------------------------------------------------|-------------|
| <b>Capital Investment, USD</b>                          | 558,361,860 |
| <b>Fixed Costs, USD/year</b>                            | 48,333,340  |
| <b>Variable Costs, USD/year</b>                         | 115,817,854 |
| <b>Income corporate tax at the end of 1st year, USD</b> | 51,516,507  |

### 7.6.3 Estimation of Other Economic Factors

Several assumptions were made to perform a comprehensive economic analysis. The corporate tax rate in Kazakhstan is 20%. For this analysis, an inflation rate of 9.8% was projected for the 8-year operational period from 2028 to 2036. The Net Present Value (NPV), Internal Rate of Return (IRR), and Payback Period were calculated considering a depreciation period of 20 years.

Based on the cumulative free cash flow, the plant's economic indicators suggest strong financial viability. The NPV is estimated at 1,243,981,486 USD with an IRR of 46.44%. The payback period is projected to be 5.668 years. These values, reflecting the end of the 2026 and 2036 periods, are detailed in Tables 57 and 58.

**Table 57.** Comparison of economic indicators for the end of 2026 and 2034.

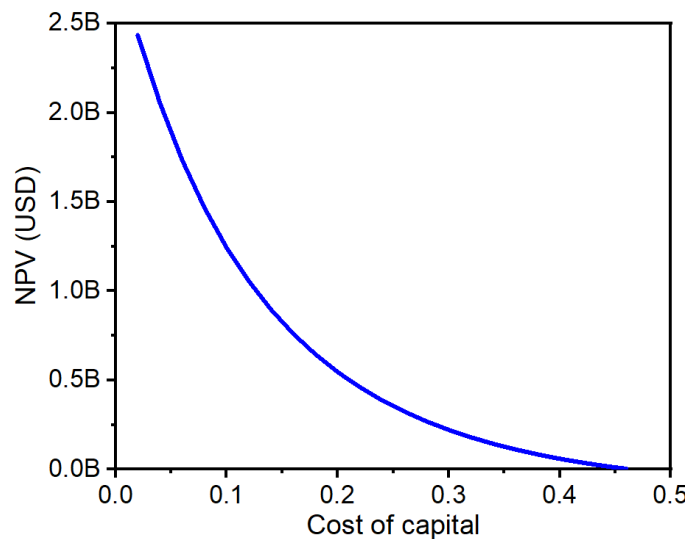
| <b>Economic indicator</b>    | <b>2028</b> | <b>2036</b> |
|------------------------------|-------------|-------------|
| <b>Revenue</b>               | 441,436,475 | 932,581,801 |
| <b>Cost of Raw Materials</b> | 101,987,824 | 215,460,194 |
| <b>Total fixed cost</b>      | 53,070,008  | 112,116,071 |
| <b>Utility Cost</b>          | 24,706,696  | 52,195,539  |
| <b>Gross Profit</b>          | 339,448,651 | 717,121,607 |
| <b>Unlevered Income</b>      | 258,056,023 | 549,720,874 |

**Table 58.** Major economic indicator for the ethylene production plant

| <b>Economic indicator</b> | <b>Values</b>     |
|---------------------------|-------------------|
| <b>Payback period</b>     | 5.668 years       |
| <b>NPV, USD dollars</b>   | 1,243,981,486 USD |
| <b>IRR, %</b>             | 46.44%            |

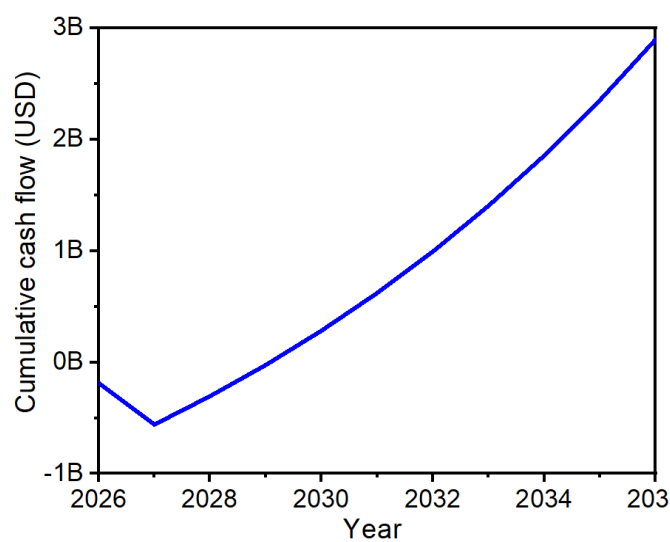
Figure 16 illustrates the relationship between Net Present Value (NPV) and the cost of capital. As the cost of capital increases, the NPV decreases, following a classic downward-sloping curve. The graph shows that at low levels of cost of capital (around 0 to 0.10), the NPV is significantly positive, indicating a profitable investment. However, as the cost of capital rises beyond 0.10, the NPV decreases progressively, approaching zero. Eventually, at higher values of the cost of capital (approaching 0.50), the NPV becomes negative, signaling that the investment would result in a loss. This figure highlights the critical importance of managing

the cost of capital to ensure the profitability of a project, as higher financing costs erode the value generated by the project.



**Figure 16.** NPV vs. Cost of capital

Figure 17 illustrates the project's financial lifecycle, beginning with a capital investment phase from 2026 to 2027 where cumulative cash flow drops to a deficit of approximately \$0.5B. Following this initial spend, the project enters a recovery period, eventually reaching its break-even point around 2030 when the blue line crosses the zero axis. From 2030 onward, the project shows strong, accelerating profitability, ultimately reaching a cumulative surplus of nearly \$3B by the end of the timeline. The upward-curving slope indicates that the project's annual earnings are increasing over time, making it a long-term growth asset once the initial four-year payback period is cleared.



**Figure 17.** Cumulative cash flow vs. Year

## Chapter 8. Conclusions and Future Work

### *8.1 Conclusions and Future Work*

This capstone project presents a comprehensive and fully integrated design for a 220 kta ethylene production plant targeting 99.9% product purity. At this production rate, the plant is estimated to satisfy approximately 25% of the regional demand within the Commonwealth of Independent States (CIS) by 2028. The design is grounded in a rigorous comparative analysis of four industrial production routes - steam cracking of natural gas, ethanol dehydration, methanol-to-olefins, and oxidative coupling of methane. Steam cracking of ethane was selected as the most suitable pathway due to Kazakhstan's abundant natural gas reserves, the maturity of the technology, its comparatively low production cost of approximately 832 USD per tonne of ethylene, and the well-established availability of kinetic and operational data.

The core reaction section comprises a tubular plug-flow reactor (H-101) housed within a gas-fired furnace, operating at 850°C and 4 bar. An ethane conversion of 65% was targeted to optimize ethylene yield while limiting coke formation and side reactions. The reaction kinetics were modeled, with five reactions. The reactor was designed with 72 parallel tubes of Incoloy 800H alloy, selected for its superior creep rupture strength and long-term microstructural stability above 800°C, yielding a total reactor volume of 3.577 m<sup>3</sup> and a heat duty of approximately 70.83 MW. Pressure drop across the reactor coil was confirmed to be negligible at 0.0102 bar using three independent calculation methods.

The separation train incorporates a quench tower and molecular sieve dryer for water removal, a multi-stage compressor train raising pressure progressively to 20 bar, and a sequence of three packed distillation columns. The demethanizer T-101 removes hydrogen and methane overhead, the de-ethanizer T-102 isolates C<sub>2</sub> fractions from heavier components, and the C<sub>2</sub> splitter T-103, the most demanding separation unit with 128 stages and a reflux ratio of 4.37, delivers polymer-grade ethylene at 99.9% purity. An acetylene hydrogenation reactor H-102 was incorporated between the de-ethanizer and the splitter to resolve the near-identical relative volatilities of acetylene and ethane that would otherwise prevent clean separation. All distillation columns utilize 38 mm Pall ring packing in stainless steel 316L, with designs validated against Aspen Plus RadFrac simulations.

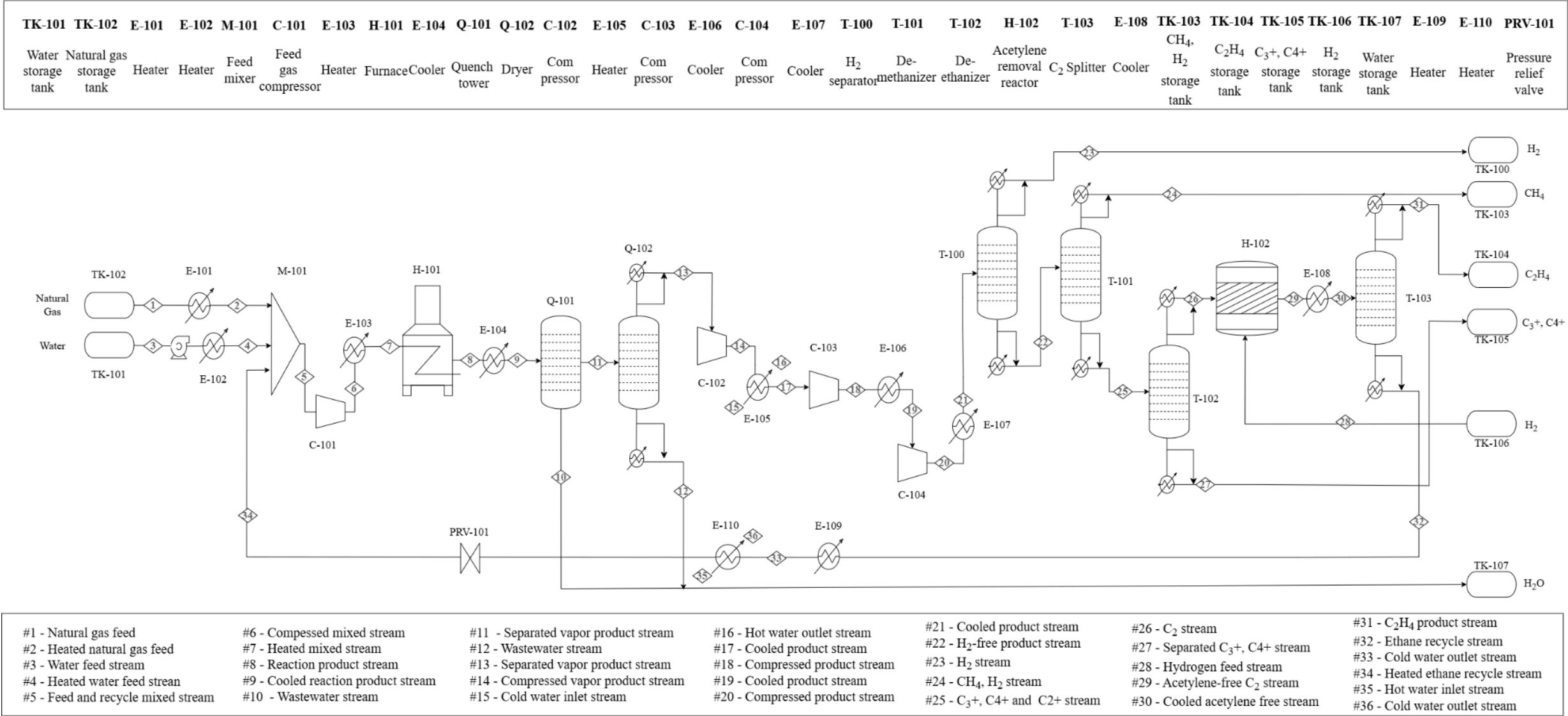
Detailed specifications for both major and minor equipment were developed in this project, including shell-and-tube heat exchangers E-105 and E-110 designed to TEMA BEM standards, four compressor units, a quench tower, a zeolite 3A molecular sieve dryer, and seven storage tanks sized for 30 days of continuous operation.

The plant location within the Karabatan National Industrial Petrochemical Technopark (NIPT) Special Economic Zone in the Atyrau Region was strategically selected for its direct access to major natural gas pipeline routes supplying feedstock from the Tengiz, Kashagan, and

Karachaganak fields, its well-developed transport infrastructure including road and rail connections, reliable utilities including a 310 MW on-site power plant and 15,000 m<sup>3</sup>/day water treatment capacity, and its proximity to the emerging Silleno polyethylene project as a primary off-taker. Environmental compliance is addressed through continuous emission monitoring systems, low-NO<sub>x</sub> burners, selective catalytic reduction, thermal oxidation of VOCs, and reverse osmosis treatment of the wastewater stream. Total combined greenhouse gas emissions were estimated at approximately 478,948 tonnes per year, with mitigation pathways identified including carbon capture and utilization and integration of low-carbon fuel sources.

From an economic perspective, capital investments, fixed costs, and variable costs were thoroughly analyzed using Aspen Process Economic Analyzer, Capcost 2017, and manual calculations. The total capital investment is estimated at USD 558,361,860. Annual fixed costs are approximately USD 48,333,340 and annual variable costs are approximately USD 115,817,854, driven primarily by water as a raw material and utility consumption. Total annual revenue from ethylene and hydrogen sales is projected at USD 402,036,862, with ethylene contributing approximately 87.3% of this figure at an assumed selling price of 1,450 USD per tonne. The project demonstrates a Net Present Value of USD 1,243,981,486, an Internal Rate of Return of 46.44%, and a payback period of 5.668 years over the 2028-2036 operational period. These metrics confirm the project's strong financial viability and its strategic relevance to Kazakhstan's petrochemical sector development and regional market positioning.

Future work should address several areas to strengthen and extend this design. First, a full dynamic simulation and control system design should be developed to evaluate transient start-up, shutdown, and disturbance rejection behavior, particularly for the high-pressure cryogenic separation section. Second, a detailed coking model for the H-101 furnace tubes should be incorporated to predict decoking cycle frequency and its impact on plant availability and maintenance scheduling. Third, all minor units need a detailed design, including, pumps, heat exchangers and a dehydrogenation unit. Fourth, the economic analysis could be refined by incorporating a sensitivity analysis of ethylene selling price, natural gas feedstock cost, and discount rate to better characterize project risk under volatile market conditions. Finally, integration opportunities with the adjacent Silleno polyethylene project should be explored, as direct ethylene pipeline supply could eliminate storage and compression costs, significantly improving the overall value chain economics.



|                                |                    |
|--------------------------------|--------------------|
| Target production rate, kmol/h | 961.06             |
| Feed                           | Molar rate, kmol/h |
| Natural gas                    | 1600.0             |
| Steam                          | 750.00             |

| Compound | Molecular weight |
|----------|------------------|
| C2H6     | 30.06964         |
| C2H4     | 28.05376         |
| H2       | 2.01588          |
| C3H8     | 44.09652         |
| C2H2     | 26.03788         |
| C4H6     | 54.09164         |
| C3H6     | 42.08064         |
| H2O      | 18.01528         |

|                   |       |
|-------------------|-------|
| IN                | 60988 |
| OUT               | 60988 |
| Ethylene produced | 27615 |

| Aspen mass rate (kg/h) |         |         |         |         |           |           |           |         |            |            |            |            |           |           |           |         |         |
|------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|------------|------------|------------|------------|-----------|-----------|-----------|---------|---------|
| Stream                 | 1       | 2       | 3       | 4       | 5         | 6         | 7         | 8       | 9          | 10         | 11         | 12         | 13        | 14        | 15        | 16      | 17      |
| Temperature, C         | 25.00   | 100.00  | 25.00   | 101.54  | 95.67     | 205.27    | 850.00    | 850.00  | 200.00     | 40.00      | 40.00      | 40.00      | 40.00     | 99.41     | 25.00     | 40.12   | 40.00   |
| Pressure, bar          | 1.00    | 1.00    | 1.00    | 1.00    | 1.00      | 1.00      | 4.00      | 4.00    | 3.99       | 4.00       | 4.00       | 4.00       | 4.00      | 10.00     | 1.00      | 10.00   | 15.00   |
| Vapor fraction         | 1.00    | 1.00    | 0.00    | 1.00    | 1.00      | 1.00      | 1.00      | 1.00    | 1.00       | 0.00       | 1.00       | 0.01       | 1.00      | 1.00      | 0.00      | 0.00    | 1.00    |
| Mass flow rates (kg/h) |         |         |         |         |           |           |           |         |            |            |            |            |           |           |           |         |         |
| CH4                    | 1026.7  | 1026.7  | 0.0     | 0.0     | 1026.7    | 1026.7    | 1026.7    | 6828.3  | 0.0066061  | 6828.3     | 0.68283    | 6827.6     | 6827.6    | 0         | 0         | 6827.6  | 6827.6  |
| C3H8                   | 705.54  | 705.54  | 0.00    | 0.00    | 708.01    | 708.01    | 708.01    | 1321.4  | 0.00018662 | 1321.4     | 0.13214    | 1321.2     | 1321.2    | 0         | 0         | 1321.2  | 1321.2  |
| C2H4                   | 0       | 0       | 0       | 0       | 5424.5    | 5424.5    | 5424.5    | 32992   | 0.049944   | 32992      | 3.2992     | 32989      | 32989     | 0         | 0         | 32989   | 32989   |
| C3H6                   | 0       | 0       | 0       | 0       | 298.11    | 298.11    | 298.11    | 882.10  | 0.00046035 | 882.10     | 0.08821    | 882.01     | 882.01    | 0         | 0         | 882.01  | 882.01  |
| H2                     | 0       | 0       | 0       | 0       | 0         | 0         | 0         | 2656.2  | 0.00047667 | 2656.2     | 0.26562    | 2656.0     | 2656.0    | 0         | 0         | 2656.0  | 2656.0  |
| C2H6                   | 45706   | 45706   | 0       | 0       | 72111     | 72111     | 72111     | 26216   | 0.027250   | 26216      | 2.6216     | 26214      | 26214     | 0         | 0         | 26214   | 26214   |
| H2O                    | 0       | 0       | 13511   | 13511   | 13511     | 13511     | 13511     | 13511   | 12313      | 1198.4     | 1198.2     | 0.11984    | 0.11984   | 159027    | 159027    | 0.11984 | 0.11984 |
| C2H2                   | 0       | 0       | 0       | 0       | 0.0017655 | 0.0017655 | 0.0017655 | 331.61  | 0.0050882  | 331.61     | 0.033161   | 331.58     | 331.58    | 0         | 0         | 331.58  | 331.58  |
| C4H6                   | 0       | 0       | 0       | 0       | 0         | 0         | 0         | 8340.2  | 0.0022397  | 8340.2     | 0.83402    | 8339.4     | 8339.4    | 0         | 0         | 8339.4  | 8339.4  |
| Total                  | 47438   | 47438   | 13511   | 13511   | 93080     | 93080     | 93080     | 93080   | 93080      | 12313      | 80766      | 1206.2     | 79560     | 79560     | 159027    | 159027  | 79560   |
| Stream                 | 19      | 20      | 21      | 22      | 23        | 24        | 25        | 26      | 27         | 28         | 29         | 30         | 31        | 32        | 33        | 34      | 35      |
| Temperature, C         | 40.00   | 65.02   | -107.57 | -107.57 | -107.57   | -106.84   | -16.77    | -19.51  | 92.39      | 60.00      | 60.00      | -29.12     | -29.61    | -12.02    | 20.00     | 100.00  | 150.00  |
| Pressure, bar          | 15.00   | 20.00   | 20.00   | 20.00   | 20.00     | 19.94     | 20.00     | 19.85   | 20.00      | 20.00      | 20.00      | 19.64      | 19.64     | 20.00     | 20.00     | 20.00   | 1.00    |
| Vapor fraction         | 1.00    | 1.00    | 0.38    | 0.00    | 1.00      | 1.00      | 0.00      | 1.00    | 0.00       | 1.00       | 1.00       | 0.00       | 1.00      | 0.00      | 1.00      | 1.00    | 0.97    |
| Mass flow rates (kg/h) |         |         |         |         |           |           |           |         |            |            |            |            |           |           |           |         |         |
| CH4                    | 6827.6  | 6827.6  | 6827.6  | 6827.6  | 0         | 6816.5    | 11.133    | 0       | 0          | 11.132     | 11.132     | 11.132     | 0         | 0         | 0         | 0       | 0       |
| C3H8                   | 1321.2  | 1321.2  | 1321.2  | 1321.2  | 0         | 0         | 1321.2    | 2.4703  | 1318.8     | 0          | 2.4705     | 2.4705     | 0         | 2.4705    | 2.4705    | 2.4705  | 0       |
| C2H4                   | 32989   | 32989   | 32989   | 32989   | 0         | 127.99    | 32861     | 0       | 0          | 33039      | 33039      | 27615      | 5424.5    | 5424.5    | 5424.5    | 0       | 0       |
| C3H6                   | 882.01  | 882.01  | 882.01  | 882.01  | 0         | 0         | 882.01    | 298.11  | 583.90     | 0          | 298.11     | 298.11     | 0         | 298.11    | 298.11    | 298.11  | 0       |
| H2                     | 2656.0  | 2656.0  | 2656.0  | 2.6560  | 2653.3    | 2.6560    | 0         | 0       | 38.484     | 0.00038484 | 0.00038484 | 0.00038484 | 0         | 0         | 0         | 0       | 0       |
| C2H6                   | 26214   | 26214   | 26214   | 26214   | 0         | 0.10764   | 26214     | 26214   | 0          | 0          | 26405      | 26405      | 0.085470  | 26405     | 26405     | 26405   | 0       |
| H2O                    | 0.11984 | 0.11984 | 0.11984 | 0.11984 | 0         | 0         | 0.11984   | 0       | 0.11984    | 0          | 0          | 0          | 0         | 0         | 0         | 0       | 28659   |
| C2H2                   | 331.58  | 331.58  | 331.58  | 331.58  | 0         | 0.19009   | 331.39    | 331.39  | 0          | 0.0033139  | 0.0033139  | 0.0015483  | 0.0017655 | 0.0017655 | 0.0017655 | 0       | 0       |
| C4H6                   | 8339.4  | 8339.4  | 8339.4  | 8339.4  | 0         | 0         | 8339.4    | 0       | 8339.4     | 0          | 0          | 0          | 0         | 0         | 0         | 0       | 0       |
| Total                  | 79560   | 79560   | 79560   | 76907   | 2653.3    | 6947.4    | 69959     | 59717   | 10242      | 38.484     | 59756      | 59756      | 27626     | 32130     | 32130     | 32130   | 28659   |
| Stream                 | 36      | 37      | 38      | 39      | 40        | 41        | 42        | 43      | 44         | 45         | 46         | 47         | 48        | 49        | 50        | 51      | 52      |
| Temperature, C         | 101.54  | 150.00  | 101.54  | 101.54  | 101.54    | 101.54    | 101.54    | 101.54  | 101.54     | 101.54     | 101.54     | 101.54     | 101.54    | 101.54    | 101.54    | 101.54  | 101.54  |
| Pressure, bar          | 1.00    | 1.00    | 1.00    | 1.00    | 1.00      | 1.00      | 1.00      | 1.00    | 1.00       | 1.00       | 1.00       | 1.00       | 1.00      | 1.00      | 1.00      | 1.00    | 1.00    |
| Vapor fraction         | 1.00    | 1.00    | 1.00    | 1.00    | 1.00      | 1.00      | 1.00      | 1.00    | 1.00       | 1.00       | 1.00       | 1.00       | 1.00      | 1.00      | 1.00      | 1.00    | 1.00    |
| Mass flow rates (kg/h) |         |         |         |         |           |           |           |         |            |            |            |            |           |           |           |         |         |
| CH4                    | 6827.6  | 6827.6  | 6827.6  | 6827.6  | 6827.6    | 6827.6    | 6827.6    | 6827.6  | 6827.6     | 6827.6     | 6827.6     | 6827.6     | 6827.6    | 6827.6    | 6827.6    | 6827.6  | 6827.6  |
| C3H8                   | 1321.2  | 1321.2  | 1321.2  | 1321.2  | 1321.2    | 1321.2    | 1321.2    | 1321.2  | 1321.2     | 1321.2     | 1321.2     | 1321.2     | 1321.2    | 1321.2    | 1321.2    | 1321.2  | 1321.2  |
| C2H4                   | 32989   | 32989   | 32989   | 32989   | 32989     | 32989     | 32989     | 32989   | 32989      | 32989      | 32989      | 32989      | 32989     | 32989     | 32989     | 32989   | 32989   |
| C3H6                   | 882.01  | 882.01  | 882.01  | 882.01  | 882.01    | 882.01    | 882.01    | 882.01  | 882.01     | 882.01     | 882.01     | 882.01     | 882.01    | 882.01    | 882.01    | 882.01  | 882.01  |
| H2                     | 2656.0  | 2656.0  | 2656.0  | 2656.0  | 2656.0    | 2656.0    | 2656.0    | 2656.0  | 2656.0     | 2656.0     | 2656.0     | 2656.0     | 2656.0    | 2656.0    | 2656.0    | 2656.0  | 2656.0  |
| C2H6                   | 26214   | 26214   | 26214   | 26214   | 26214     | 26214     | 26214     | 26214   | 26214      | 26214      | 26214      | 26214      | 26214     | 26214     | 26214     | 26214   | 26214   |
| H2O                    | 0.11984 | 0.11984 | 0.11984 | 0.11984 | 0.11984   | 0.11984   | 0.11984   | 0.11984 | 0.11984    | 0.11984    | 0.11984    | 0.11984    | 0.11984   | 0.11984   | 0.11984   | 0.11984 | 0.11984 |
| C2H2                   | 331.58  | 331.58  | 331.58  | 331.58  | 331.58    | 331.58    | 331.58    | 331.58  | 331.58     | 331.58     | 331.58     | 331.58     | 331.58    | 331.58    | 331.58    | 331.58  | 331.58  |
| C4H6                   | 8339.4  | 8339.4  | 8339.4  | 8339.4  | 8339.4    | 8339.4    | 8339.4    | 8339.4  | 8339.4     | 8339.4     | 8339.4     | 8339.4     | 8339.4    | 8339.4    | 8339.4    | 8339.4  | 8339.4  |
| Total                  | 79560   | 79560   | 79560   | 79560   | 79560     | 79560     | 79560     | 79560   | 79560      | 79560      | 79560      | 79560      | 79560     | 79560     | 79560     | 79560   | 79560   |

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## Appendix A - Production Rate Determination

**Table A1.** Ethylene production in China [1]

| Year | Production Capacity | Capacity * Scaling factor |
|------|---------------------|---------------------------|
| 2007 | 10278               | 305.3                     |
| 2008 | 9876                | 293.3                     |
| 2009 | 10726               | 318.6                     |
| 2010 | 14213               | 422.1                     |
| 2011 | 15275               | 453.7                     |
| 2012 | 14868               | 441.6                     |
| 2013 | 15993               | 475.0                     |
| 2014 | 169687              | 503.9                     |
| 2015 | 17146               | 509.2                     |
| 2016 | 17811               | 529.0                     |
| 2017 | 18218               | 541.1                     |
| 2018 | 18410               | 546.8                     |

### 1. Calculation of the scaling factor

$$\text{scaling factor} = \frac{\text{GDP of CIS countries}}{\text{GDP of China}} \quad (1)$$

$$\text{scaling factor} = \frac{421 \text{ billion USD}}{14,150 \text{ billion USD}} = 0.0297$$

### 2. Calculation of ethylene market in CIS region

$$\text{ethylene market in CIS} = 18,410 \text{ kta} \times 0.0297 = 546.777 \text{ kta}$$

### 3. Calculation of the total production rate

$$\text{production rate} = 816.2 \text{ kta} \times 0.25 = 204 \text{ kta}$$

## Appendix B - Reaction Kinetics

### 1. Rate expressions derivation

$$r_i = k_i \prod_j C_j \quad (2)$$

Where,

$$k_i = A e^{-E_a/RT} \quad (3)$$

$$C_j = \left(\frac{F_j}{F_T}\right) \left(\frac{P}{RT}\right) \quad (4)$$

$$F_T = F_{steam} + \sum_j F_j \quad (5)$$

The rate expressions were derived by Froment et al [2]. Using Eq. (9), the rate expressions were derived in terms of concentrations. The first reaction of ethane dehydrogenation is taken as an example:

$$r_1 = k_1 \left[ \frac{F_{ETH}}{F_T} \left( \frac{P_t}{TR} \right) - \frac{F_{ETLN} F_{HRG}}{F_T^2 K_{C1}} \left( \frac{P_T}{RT} \right)^2 \right] \quad (6)$$

Which results in:

$$\mathbf{R1:} \quad r_1 = k_1 (C_{ETH} - \frac{C_{ETLN}^* C_{HRG}}{K_{C1}}) \quad (7)$$

Reactions R2-R5 were derived in the same manner.

$$\mathbf{R2:} \quad r_2 = k_2 C_{ETH} \quad (8)$$

$$\mathbf{R3:} \quad r_3 = k_3 (C_{PRO} - \frac{C_{ACT}^* C_{MET}}{K_{C2}}) \quad (9)$$

$$\mathbf{R4:} \quad r_4 = k_4 (C_{ACT} C_{ETLN}) \quad (10)$$

$$\mathbf{R5:} \quad r_5 = k_5 (C_{ETH} C_{ETLN}) \quad (11)$$

### 2. Steady-state continuity equations

The continuity equations for the components can be written as [2]:

$$\frac{dF_j}{dV} = - \sum_{i=1}^{N_r} s_{ji} r_i \quad (12)$$

Where  $s_{ij}$  represents the stoichiometric coefficient for the  $j$ th component in the  $i$ th reaction.

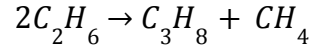
The rate of ethane consumption can be expressed as the sum of the rates of reactions R1, R2, and R5.

$$r_{ETH} = r_{R1} + r_{R2} + r_{R5} \quad (13)$$

Combining Eq. 12 and 13, the steady-state continuity equation for ethane becomes:

$$\frac{dF_{ETH}}{dV} = -r_1 - 2r_2 - r_5 \quad (14)$$

Where the coefficient of 2 appears before  $r_2$  as two moles of ethane are consumed in R2:



The continuity equations for other components were derived likewise.

$$\frac{dF_{ETLN}}{dV} = r_1 + r_2 - r_4 - r_5 \quad (15)$$

$$\frac{dF_{HRG}}{dV} = r_1 \quad (16)$$

$$\frac{dF_{MET}}{dV} = 2r_2 + r_3 + r_5 \quad (17)$$

$$\frac{dF_{PRLN}}{dV} = -r_3 + r_5 \quad (18)$$

$$\frac{dF_{PRO}}{dV} = r_2 \quad (19)$$

$$\frac{dF_{ACT}}{dV} = r_3 - r_4 \quad (20)$$

$$\frac{dF_{BDN}}{dV} = r_4 \quad (21)$$

### 3. Reversible reactions

The reversible reactions were expressed as 2 separate reactions (forward and reverse) in order to be put as Power Law into Aspen Plus.

**Table B1.** Main and side reactions for the process with products[2]

|           | Reaction                                    | Product(s)            | Type |
|-----------|---------------------------------------------|-----------------------|------|
| <b>R1</b> | $C_2H_6 \leftrightarrow C_2H_4 + H_2$       | Ethylene and hydrogen | Main |
| <b>R2</b> | $2C_2H_6 \rightarrow C_3H_8 + CH_4$         | Propane and methane   | Side |
| <b>R3</b> | $C_3H_6 \leftrightarrow C_2H_2 + CH_4$      | Acetylene and methane | Side |
| <b>R4</b> | $C_2H_2 + C_2H_4 \rightarrow C_4H_6$        | 1,3 - butadiene       | Side |
| <b>R5</b> | $C_2H_4 + C_2H_6 \rightarrow C_3H_6 + CH_4$ | Propylene and methane | Side |

**Table B2.** Arrhenius parameters for ethane cracking Model III [2]

| Rate coefficient | A (sec <sup>-1</sup> )   | Ea (kcal/mol) |
|------------------|--------------------------|---------------|
| k <sub>1</sub>   | 4.652 * 10 <sup>13</sup> | 65.20         |
| k <sub>2</sub>   | 3.850 * 10 <sup>11</sup> | 65.25         |
| k <sub>3</sub>   | 9.814 * 10 <sup>8</sup>  | 36.92         |
| k <sub>4</sub>   | 1.026 * 10 <sup>12</sup> | 41.26         |
| k <sub>5</sub>   | 7.083 * 10 <sup>13</sup> | 60.43         |

**Table B3.** Equilibrium constants [2]

| T (°C)                  | 775                      | 800                      | 825                      |
|-------------------------|--------------------------|--------------------------|--------------------------|
| K <sub>C1</sub> (mol/L) | 8.895 * 10 <sup>-3</sup> | 1.276 * 10 <sup>-2</sup> | 1.800 * 10 <sup>-2</sup> |
| K <sub>C2</sub> (mol/L) | 9.847 * 10 <sup>-3</sup> | 1.375 * 10 <sup>-2</sup> | 1.890 * 10 <sup>-2</sup> |

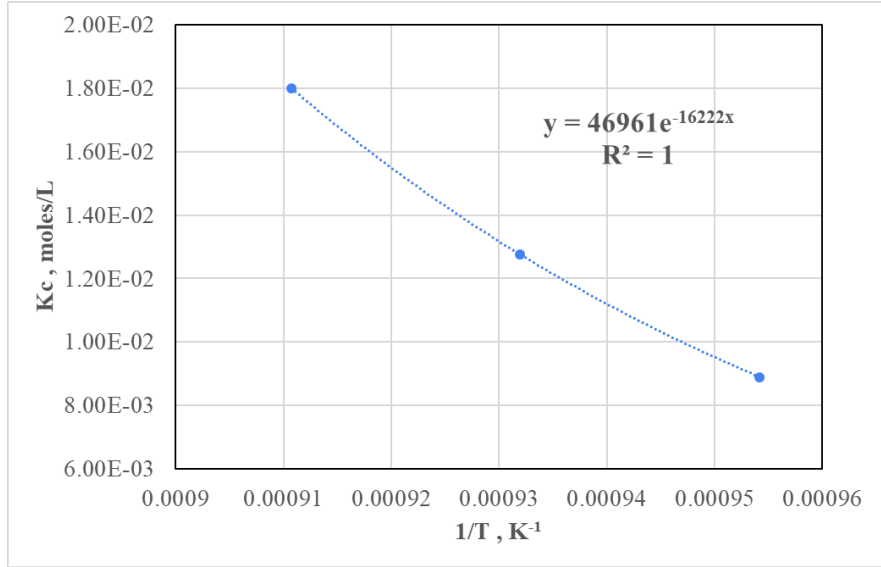
**R1 reaction:**

$$k' = \frac{A}{A(Kc1)} = \frac{4.65E+13}{46961} = 9.91 * 10^8 \text{ sec}^{-1}$$

$$E'_a = \frac{-E_{a1}/RT}{-E_{a(Kc1)}/RT} = E_{a1} - E_{a(Kc1)}$$

$$E_{a(Kc1)} = \frac{16222}{4184} * R * \frac{kcal}{J} = 32.23463384 \text{ kcal/mole}$$

$$E'_a = E_{a1} - E_{a(Kc1)} = 65.2 - 32.2 = 33.0 \text{ kcal/mole}$$



**Figure B1.** Exponential equation for Kc1

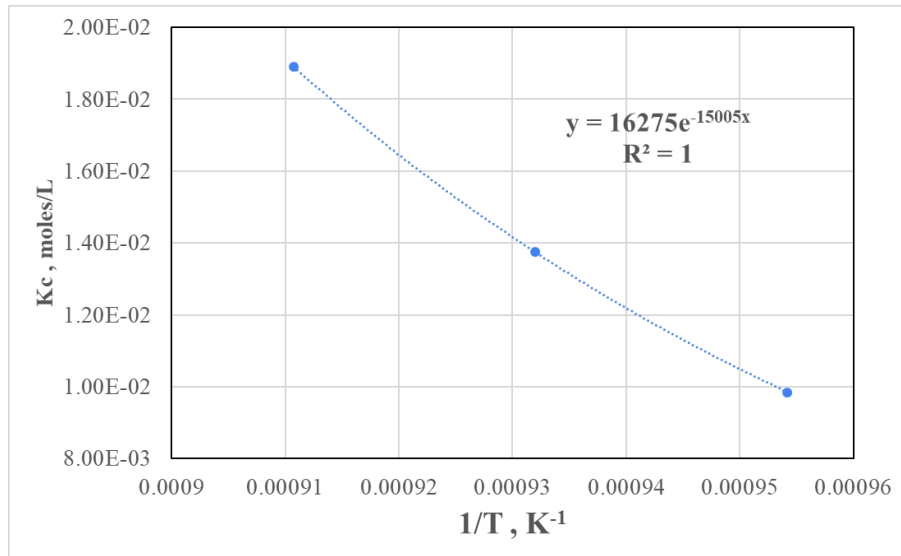
**R3 reaction:**

$$k'' = \frac{A}{A(Kc2)} = \frac{9.81E+08}{16275} = 6.03E + 04 \text{ sec}^{-1}$$

$$E_a'' = \frac{-E_{a3}/RT}{-E_{a(Kc2)}/RT} = E_{a3} - E_{a(Kc2)}$$

$$E_{a(Kc2)} = \frac{15005}{4184} * R * \frac{\text{kcal}}{J} = 29.81634082 \text{ kcal/mole}$$

$$E_a'' = E_{a3} - E_{a(Kc2)} = 36.92 - 29.82 = 7.1 \text{ kcal/mole}$$



**Figure B2.** Exponential equation for Kc2

## Appendix C - Reactor Design Sizing

### A. Reactor Sizing

#### 1. Tubes

Volumetric flowrate was taken from Aspen Plus simulation and turned into desired units. The tube size parameters were taken from ASME specifications for NPS 4 configuration[3]. The wall thickness of tubes was derived using the Cylindrical Shell equation from ASME B31.3[4]:

$$t = \frac{PD}{2*(SEW+PY)} + C \quad (22)$$

where  $t$  is the required wall thickness (mm),  $P$  is the design pressure (MPa),  $D$  is the pipe outside diameter (mm),  $S$  is the allowable stress at 850°C (MPa),  $E$  is the weld quality factor,  $W$  is the weld strength reduction factor,  $Y$  is the material coefficient for high-temperature service, and  $C$  is corrosion allowance.

Corrosion allowance was taken as corrosion rate in 5 years:

$$C = \text{Corrosion rate} * 5 \text{ years} \quad (23)$$

Internal diameter was calculated as:

$$ID = OD - 2t \quad (24)$$

$$ID = 88.9 - 2(5.49) = 77.9 \text{ mm}$$

The allowable stress value was interpolated from the Expected Minimum Stress-to-Rupture data in Table R.14.2-1 [5]. The allowable stress at 850°C for a 100,000-hour service life is approximately 11.1 MPa (interpolated between 11.7 MPa at 843°C and 9.0 MPa at 871°C).

The Schedule of pipes was then calculated as follows [6]:

$$Sch. = (P/[\sigma]) \times 1000 \quad (25)$$

Where  $P$  is operating pressure in MPa,  $[\sigma]$  is allowable stress under design temperature. The resulting value is 36.03, which is the closest to 40 Schedule tubes.

The volume of the reactor was calculated using the Euler iterative Python code based on the continuity equations.

**Table C1.** Wall thickness calculation and tube inside diameter derivation

| Parameter                         | Value       | Unit |
|-----------------------------------|-------------|------|
| Corrosion rate                    | 0.15        | mm/y |
| Allowable Stress, S               | 11.1        | MPa  |
| Outside diameter, $D_{outer}$     | 114.3       | mm   |
| Weld strength reduction factor. W | 1           |      |
| Coefficient of material used. Y   | 0.7         |      |
| Weld quality factor. E            | 1           |      |
| Wall thickness, t                 | 2.758787346 | mm   |
| Inside diameter, D                | 108.7824253 | mm   |
| NPS 4 SCH 40 wall thickness, t    | 6.02        | mm   |
| NPS 4 SCH 40 Inside diameter      | 102.26      | mm   |

**Table C2.** Tubes Sizing

| Parameter                  | Equation (if applicable)        | Value     |        | Unit              |
|----------------------------|---------------------------------|-----------|--------|-------------------|
|                            |                                 | In        | Out    |                   |
| Volumetric flow rate, Q    |                                 | 17.049    | 29.461 | m <sup>3</sup> /s |
| Tube inside diameter, D    |                                 | 0.10226   |        | m                 |
| Area of tube, A            | $A = \frac{\pi D^2}{4}$         | 0.0082088 |        | m <sup>2</sup>    |
| Space velocity, u          | $u = \frac{Q}{A \cdot N}$       | 29.056    | 50.208 | m/s               |
| Volume of reactor, V       |                                 | 2.2690    |        | m <sup>3</sup>    |
| Volume of tube, $V_{tube}$ | $V_{tube} = \frac{A}{L_{tube}}$ | 0.050041  |        | m <sup>3</sup>    |
| Number of tubes, N         | $N = \frac{V}{V_{tube}}$        | 71.481    |        |                   |
| Length, $L_{tube}$         |                                 | 6.0960    |        | m                 |
| Residence time, $\tau$     | $\tau = \frac{V}{Q}$            | 0.2098    | 0.1214 | s                 |

## 2. Reactor furnace

The pitch of the reactor was calculated as:

$$p = 1.5D_{outer} = 0.5 \times 0.1143 = 0.171m$$

The 72 tubes were placed in a near-rectangular grid with 8 x 9 layout. Bundle width and depth were calculated as follows:

**Table C3.** Furnace plan area

| Width                             | Depth                             |
|-----------------------------------|-----------------------------------|
| $W=(\text{columns}-1)\times p$    | $D=(\text{rows}-1)\times p$       |
| $W=(9-1)\times 0.171$             | $D=(8-1)\times 0.171$             |
| 1.37m                             | 1.20m                             |
| $1.37 + 0.4*2 = \mathbf{2.17\ m}$ | $1.20 + 0.4*2 = \mathbf{2.00\ m}$ |

The furnace height was estimated with 1m clearance from both sides, taking the tubes placed vertically in the furnace:

$$H=6.096+2.0=8.1\text{m}$$

**Table C4.** Reactor sizing

| Parameter         | Value  | Unit           |
|-------------------|--------|----------------|
| Volume of reactor | 3.577  | m <sup>3</sup> |
| Number of tubes   | 72     |                |
| Outside Diameter  | 0.1143 | m              |
| Pitch             | 0.171  | m              |
| Columns           | 9      |                |
| Rows              | 8      |                |
| Width             | 2.17   | m              |
| Depth             | 2.00   | m              |
| Height            | 8.10   | m              |

## B. Pressure Drop calculations

$$Re = \frac{\rho u D}{\mu} \quad (26)$$

$$f = 0.3164 Re^{-0.25} \quad (27)$$

$$\Delta P = f \frac{L_{tube}}{D} \frac{\rho u^2}{2} \quad (28)$$

**Table C5.** Pressure drop by hand calculation

| Parameter                     | In       | Out      | Unit              |
|-------------------------------|----------|----------|-------------------|
| Area 1 tube                   | 0.00821  |          | m <sup>2</sup>    |
| Volumetric flow rate per tube | 0.38749  | 0.66957  | m <sup>3</sup> /s |
| Superficial velocity          | 29.056   | 50.208   | m/s               |
| Density                       | 1.4098   | 0.81588  | kg/m <sup>3</sup> |
| Diameter                      | 0.10226  |          | m                 |
| Viscosity                     | 2.70E-05 | 3.19E-05 | Pa*s              |
| Length                        | 6.096    |          | m                 |
| Reynolds number               | 1.55E+05 | 1.31E+05 |                   |
| Friction factor               | 0.01594  | 0.01662  |                   |
| Pressure drop                 | 565.49   | 1018.9   | Pa                |

### C. Material Selection

Allowable stresses for Incoloy 800H, Type 309 stainless steel, and Type 310 stainless steel were extracted from creep rupture data corresponding to 100,000 h service life. The values for operating temperature of 850C were interpolated from respective material tables. Using identical operating conditions (0.4 MPa internal pressure and 114.3 mm outside diameter), the calculated minimum wall thicknesses were:

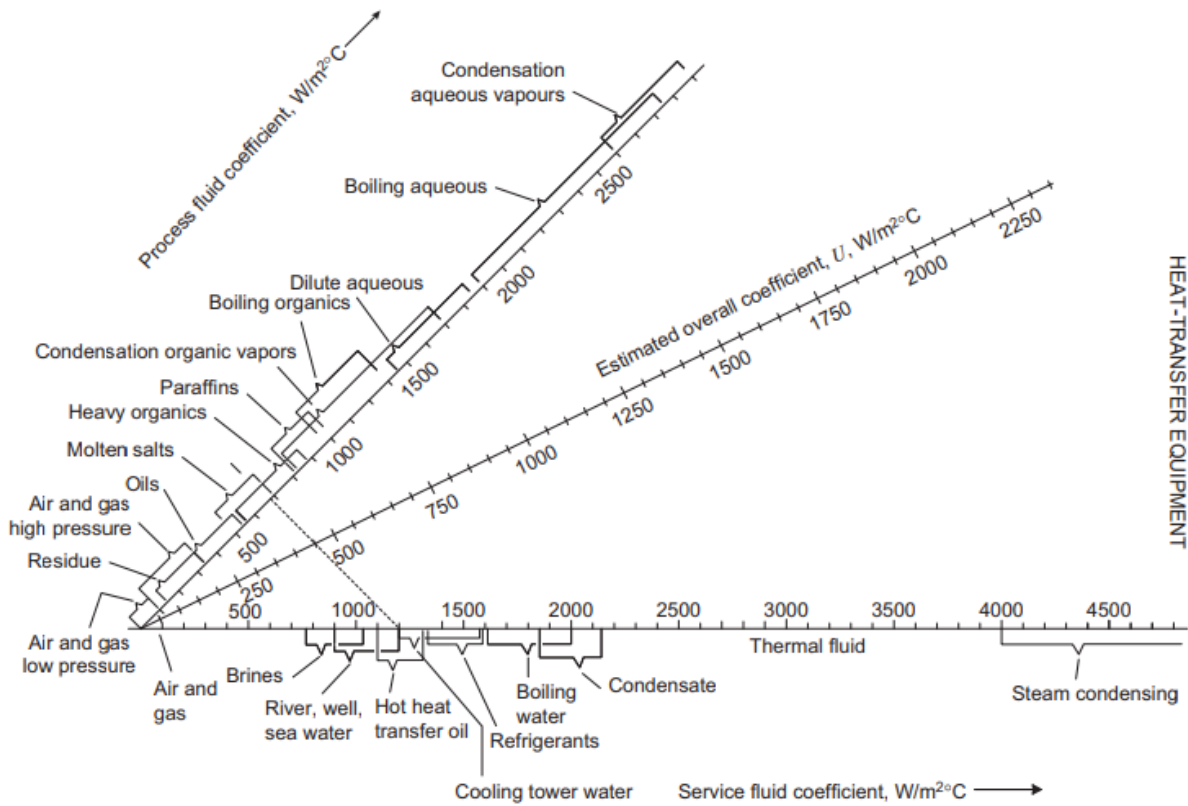
**Table C6.** Materials comparison

| Material/Property        | Incoloy 800H | SS 310  | SS 309  |
|--------------------------|--------------|---------|---------|
| Allowable stress, MPa    | 11.1[5]      | 17.5[7] | 5.25[8] |
| Corrosion rate, mm/y [5] | 0.15         | 0.23    | 2.15    |
| Wall thickness, mm       | 2.76         | 2.44    | 14.89   |

Considering that the thickness of NPS 4 SCH 40 pipes is 6.02mm, SS309 exceeds this thickness and is thus unsuitable for steam cracking coils

## Appendix D - Heat Exchanger Design

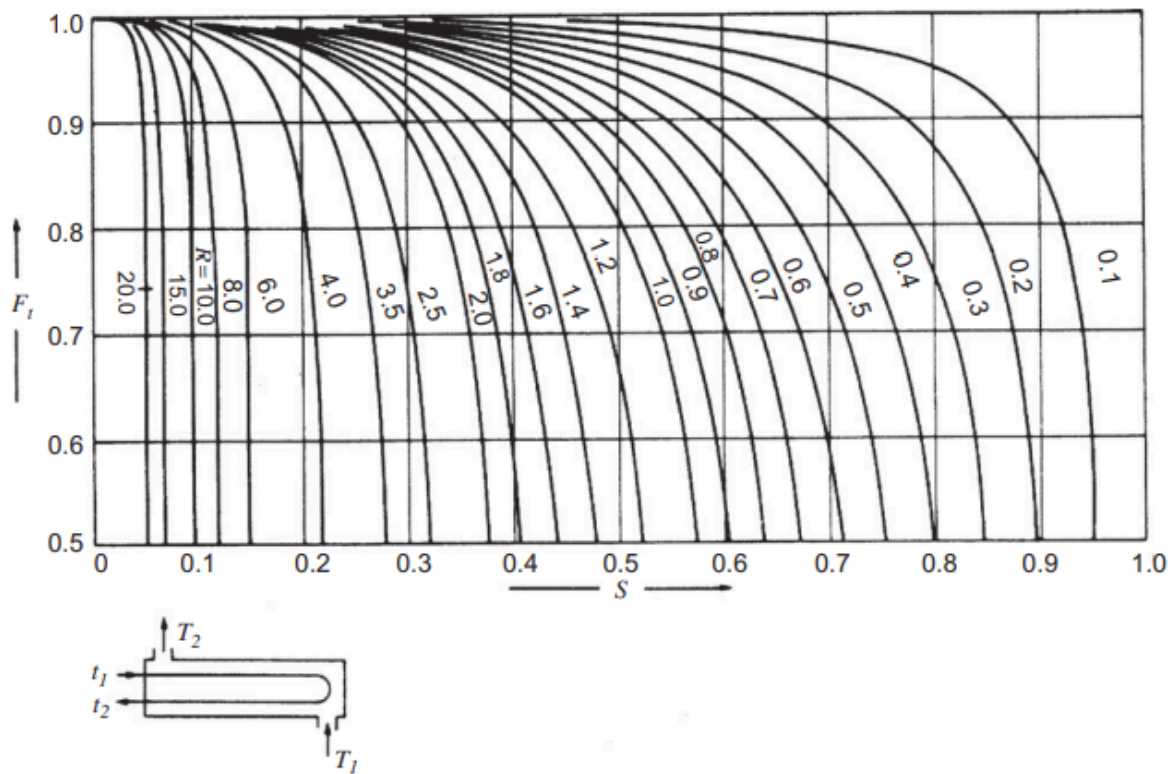
### A. TEMA specifications for tube and shell side [9]



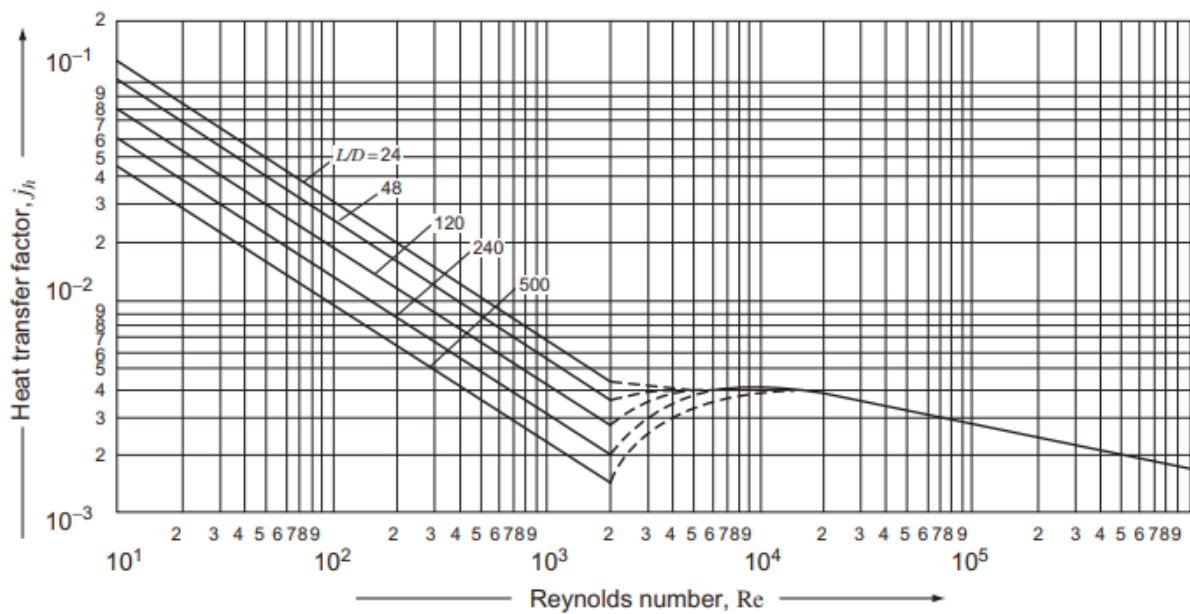
**Figure D1.** Overall U coefficients

**Table D1.** Standard Dimensions for Steel Tubes

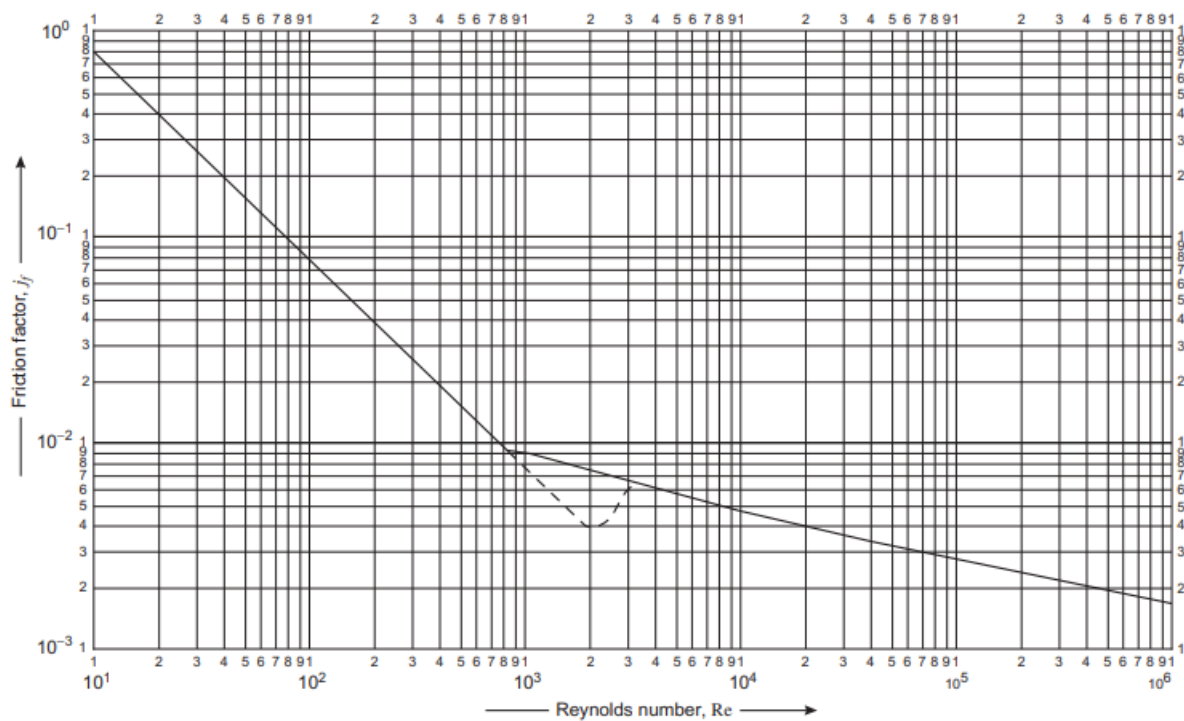
| Outside Diameter (mm) | Wall Thickness (mm) |     |     |     |     |
|-----------------------|---------------------|-----|-----|-----|-----|
| 16                    | 1.2                 | 1.7 | 2.1 | -   | -   |
| 19                    | -                   | 1.7 | 2.1 | 2.8 | -   |
| 25                    | -                   | 1.7 | 2.1 | 2.8 | 3.4 |
| 32                    | -                   | 1.7 | 2.1 | 2.8 | 3.4 |
| 38                    | -                   | -   | 2.1 | 2.8 | 3.4 |
| 50                    | -                   | -   | 2.1 | 2.8 | 3.4 |



**Figure D2.** Temperature correction factor: one shell pass, two or more even tube passes



**Figure D3.** Tube-side heat transfer factor



**Figure D4.** Tube-side friction factor

**Table D2.** Shell and tube fluid velocities

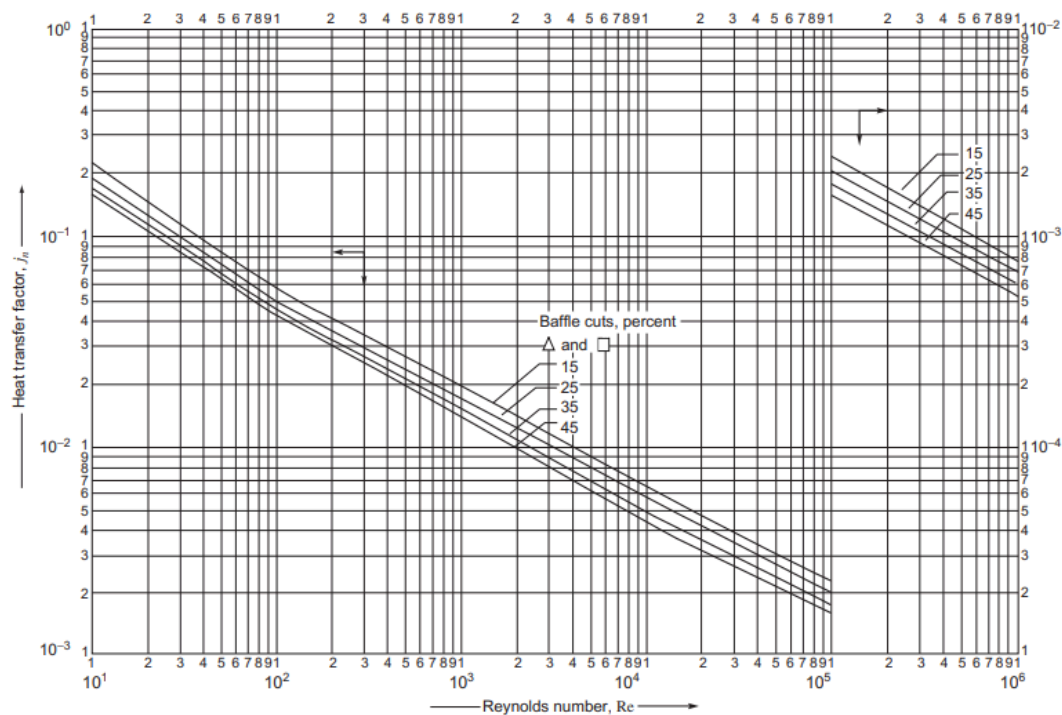
|                |                           |                |
|----------------|---------------------------|----------------|
| <b>Liquids</b> | Tube side, process fluids | 1 to 4 m/s     |
|                | Tube side, water          | 1.5 to 2.5 m/s |
|                | Shell side                | 0.3 to 1 m/s   |
| <b>Vapors</b>  | Vacuum                    | 50 to 70 m/s   |
|                | Atmospheric pressure      | 10 to 30 m/s   |
|                | High pressure             | 5 to 10 m/s    |

**Table D3.** Constants for Use in Bundle Diameter Calculations

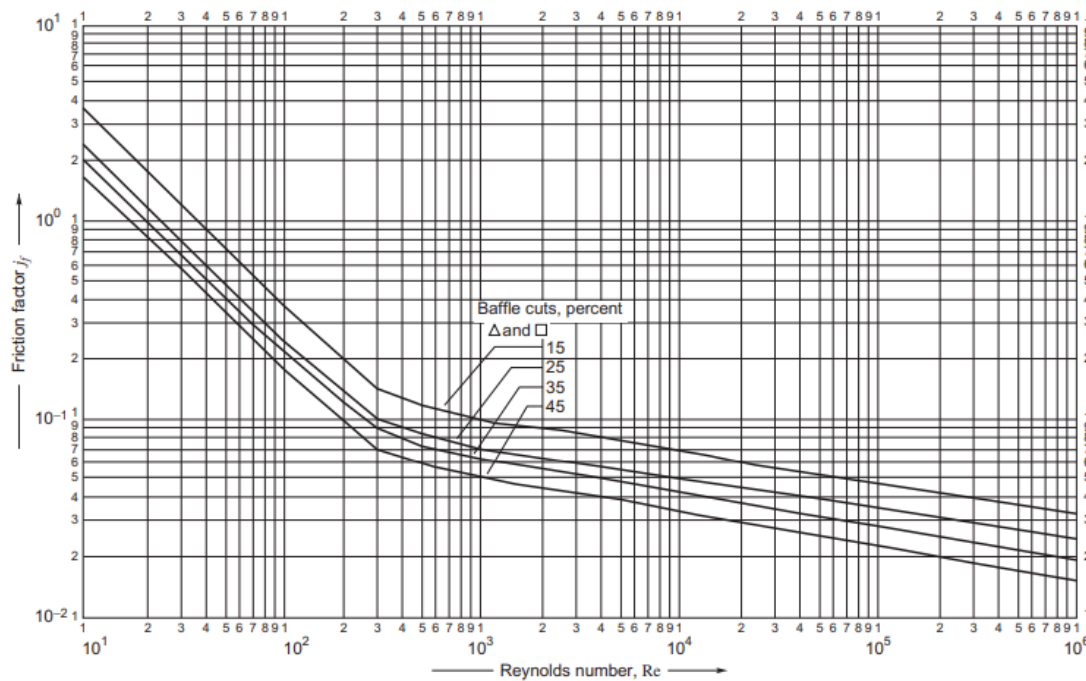
| <b>Triangular Pitch, <math>p_t = 1.25d_o</math></b> |          |          |          |          |          |
|-----------------------------------------------------|----------|----------|----------|----------|----------|
| <b>No.Passes</b>                                    | <b>1</b> | <b>2</b> | <b>3</b> | <b>4</b> | <b>5</b> |
| $K_I$                                               | 0.319    | 0.249    | 0.175    | 0.0743   | 0.0365   |
| $n_I$                                               | 2.142    | 2.207    | 2.285    | 2.499    | 2.675    |
| <b>Square Pitch, <math>p_t = 1.25d_o</math></b>     |          |          |          |          |          |
| <b>No.Passes</b>                                    | <b>1</b> | <b>2</b> | <b>3</b> | <b>4</b> | <b>5</b> |
| $K_I$                                               | 0.215    | 0.156    | 0.158    | 0.0402   | 0.0331   |
| $n_I$                                               | 2.207    | 2.291    | 2.263    | 2.617    | 2.643    |

**Table D4.** Minimum Shell thickness

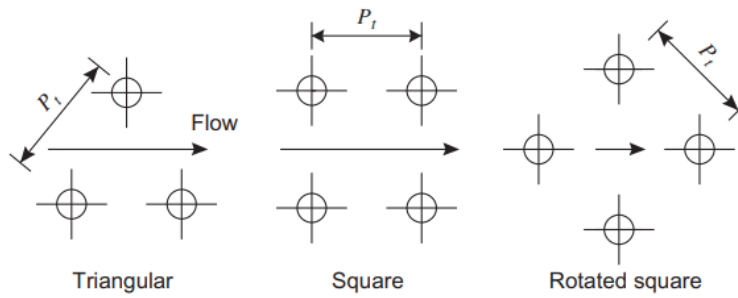
| <b>Nominal Shell Dia., mm</b> | <b>Carbon Steel</b> |              | <b>Alloy Steel</b> |
|-------------------------------|---------------------|--------------|--------------------|
|                               | <b>Pipe</b>         | <b>Plate</b> |                    |
| 150                           | 7.1                 | -            | 3.2                |
| 200-300                       | 9.3                 | -            | 3.2                |
| 330-580                       | 9.5                 | 7.9          | 3.2                |
| 610-740                       | -                   | 7.9          | 4.8                |
| 760-990                       | -                   | 9.5          | 6.4                |
| 1010-1520                     | -                   | 11.1         | 6.4                |
| 1550-2030                     | -                   | 12.7         | 7.9                |
| 2050-2540                     | -                   | 12.7         | 9.5                |



**Figure D5.** Shell-side heat-transfer factor, segmental baffles



**Figure D6.** Shell-side friction factors, segmental baffles



**Figure D7.** Tube patterns

| Metal                   | Temperature ( $^{\circ}\text{C}$ ) | $k_w(\text{W/m}^{\circ}\text{C})$ |
|-------------------------|------------------------------------|-----------------------------------|
| Aluminum                | 0                                  | 202                               |
|                         | 100                                | 206                               |
| Brass<br>(70 Cu, 30 Zn) | 0                                  | 97                                |
|                         | 100                                | 104                               |
|                         | 400                                | 116                               |
| Copper                  | 0                                  | 388                               |
|                         | 100                                | 378                               |
| Nickel                  | 0                                  | 62                                |
|                         | 212                                | 59                                |
| Cupro-nickel (10% Ni)   | 0–100                              | 45                                |
| Monel                   | 0–100                              | 30                                |
| Stainless steel (18/8)  | 0–100                              | 16                                |
| Carbon steel            | 40                                 | 60                                |
|                         | 100                                | 58                                |
|                         | 260                                | 51                                |
| Titanium                | 0–100                              | 16                                |

**Figure D8.** Conductivity of heat exchanger materials

### **Liquids**

| Viscosity                           | Allowable Pressure Drop        |
|-------------------------------------|--------------------------------|
| $<1 \text{ mN s/m}^2$               | $35 \text{ kN/m}^2$            |
| $1 \text{ to } 10 \text{ mN s/m}^2$ | $50\text{--}70 \text{ kN/m}^2$ |

### **Gas and Vapors**

|               |                                           |
|---------------|-------------------------------------------|
| High vacuum   | $0.4\text{--}0.8 \text{ kN/m}^2$          |
| Medium vacuum | $0.1 \times \text{absolute pressure}$     |
| 1 to 2 bar    | $0.5 \times \text{system gauge pressure}$ |
| Above 10 bar  | $0.1 \times \text{system gauge pressure}$ |

**Figure D9.** Allowable pressure drop values

## B. Aspen Plus Mixture Analysis Properties

**Table D5.** E-105 Natural Gas Inlet Average Properties

|                                 |          |
|---------------------------------|----------|
| Specific Heat (kJ/kg*k)         | 2.30     |
| Thermal Conductivity (kW/m*K)   | 5.53E-05 |
| Density (kg/m <sup>3</sup> )    | 7.20     |
| Viscosity (N*s/m <sup>2</sup> ) | 1.14E-05 |

**Table D6.** E-105 Water Inlet Average Properties

|                                 |          |
|---------------------------------|----------|
| Specific Heat (kJ/kg*k)         | 4.52     |
| Thermal Conductivity (kW/m*K)   | 6.10E-04 |
| Density (kg/m <sup>3</sup> )    | 993.77   |
| Viscosity (N*s/m <sup>2</sup> ) | 8.65E-04 |

**Table D7.** E-110 Recycle Stream Inlet Average Properties

|                                 |          |
|---------------------------------|----------|
| Specific Heat (kJ/kg*k)         | 2.14     |
| Thermal Conductivity (kW/m*K)   | 1.92E-05 |
| Density (kg/m <sup>3</sup> )    | 33.83    |
| Viscosity (N*s/m <sup>2</sup> ) | 9.71E-06 |

**Table D8.** E-110 Water Inlet Average Properties

|                                 |          |
|---------------------------------|----------|
| Specific Heat (kJ/kg*k)         | 4.52     |
| Thermal Conductivity (kW/m*K)   | 6.29E-04 |
| Density (kg/m <sup>3</sup> )    | 976.90   |
| Viscosity (N*s/m <sup>2</sup> ) | 6.44E-04 |

## C. Heat Transfer Correlations

Overall heat transfer coefficient:

$$\frac{1}{U_0} = \frac{1}{h_0} + \frac{1}{h_{od}} + \frac{d_o \ln\left(\frac{d_o}{d_i}\right)}{2k_w} + \frac{d_o}{d_i} \times \frac{1}{h_{id}} + \frac{d_o}{d_i} \times \frac{1}{h_i} \quad (29)$$

Where  $U_o$ = overall coefficient based on the outside area of the tube, W/m<sup>2</sup>°C

$h_o$ =outside fluid film coefficient, W/m<sup>2</sup>°C

$h_i$ = inside fluid film coefficient, W/m<sup>2</sup>°C

$h_{od}$ =outside dirt coefficient (fouling factor), W/m<sup>2</sup>°C

$h_{id}$ =inside dirt coefficient, W/m<sup>2</sup>°C

$k_w$ = thermal conductivity of the tube wall material, W/m<sup>2</sup>°C

$d_i$ = tube inside diameter, m

$d_o$ =tube outside diameter, m

R and S for the temperature correction factor F:

$$R = \frac{(T_1 - T_2)}{(t_2 - t_1)} \quad (30)$$

$$S = \frac{(t_2 - t_1)}{(T_1 - t_1)} \quad (31)$$

Where,  $T_1$ = hot fluid temperature, inlet

$T_2$ = hot fluid temperature, outlet

$t_1$ = cold fluid temperature, inlet

$t_2$ = cold fluid temperature, outlet

Fouling factor  $F_t$

$$F_t = \frac{\sqrt{(R^2 + 1)} \ln \left[ \frac{(1-S)}{(1-RS)} \right]}{(R-1) \ln \left[ \frac{2-S[R+1-\sqrt{(R^2+1)}]}{2-S[R+1+\sqrt{(R^2+1)}]} \right]} \quad (32)$$

Tube side heat transfer:

Nusselt Number:

$$Nu = C \cdot Re^{0.8} \cdot Pr^{0.33} \cdot \left( \frac{\mu}{\mu_w} \right)^{0.14} \quad (33)$$

where:

$C = 0.021$  for gases

$C = 0.023$  for nonviscous liquids

$C = 0.027$  for viscous liquids

Reynolds number:

$$Re = \frac{\rho u d_e}{\mu} = \frac{G_r d_e}{\mu} \quad (34)$$

Where,  $\rho$ = Density (kg/m<sup>3</sup>)

$u$ = Velocity (m/s)

$d_e$  = Characteristic length (m)

$\mu$ = Dynamic viscosity (Pa·s)

$G_r$  = Mass flow rate per unit area (kg/(m<sup>2</sup>·s))

Prandtl number:

$$Pr = \frac{C_p \mu}{k_f} \quad (35)$$

Inside fluid film coefficient  $h_i$ :

$$\frac{h_i d_i}{k_f} = j_h \cdot Re^{0.33} \cdot Pr^{0.33} \cdot \left( \frac{\mu}{\mu_w} \right)^{0.14} \quad (36)$$

Solved for  $h_i$ :

$$h_i = \frac{j_h \cdot Re^{0.33} \cdot Pr^{0.33} \cdot \left( \frac{\mu}{\mu_w} \right)^{0.14} \cdot k_f}{d_i} \quad (37)$$

Tube side pressure drop  $\Delta P$ :

$$\Delta P_t = N_p \left[ 8 j_f \left( \frac{L}{d_i} \right) \left( \frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2} \quad (38)$$

where,  $\Delta P_t$  = tube-side pressure drop, N/m<sup>2</sup> (Pa)

$N_p$  = number of tube-side passes

$u_t$  = tube-side velocity, m/s

$L$  = length of one tube

Shell Side Heat Transfer:

Area for cross-flow  $A_s$ :

$$A_s = \frac{(p_t - d_o) D_s l_B}{p_t} \quad (39)$$

where,  $p_t$  = tube pitch

$d_o$  = tube outside diameter

$D_s$  = shell inside diameter, m

$l_B$  = baffle spacing, m

The shell-side mass velocity  $G_s$  and the linear velocity  $u_s$ :

$$u_s = \frac{G_s}{\rho} \quad (40)$$

$$G_s = \frac{W_s}{A_s} \quad (41)$$

where,  $W_s$  = fluid flow rate on the shell-side, kg/s

$\rho$  = shell-side fluid density, kg/m<sup>3</sup>

The shell-side equivalent diameter. For a square pitch arrangement:

$$d_e = \frac{4(p_t^2 - \pi d_o^2)}{4\pi d_o} = \frac{1.27}{d_o} (p_t^2 - 0.785 d_o^2) \quad (42)$$

For an equilateral triangular pitch arrangement:

$$d_e = \frac{4\left(\frac{p_t}{2} \times 0.87 p_t - \frac{1}{2} \pi d_o^2\right)}{\pi d_o} = \frac{1.10}{d_o} (p_t^2 - 0.917 d_o^2) \quad (43)$$

where,  $d_e$  = equivalent diameter, m.

The shell-side Reynolds number,  $Re$ :

$$Re = \frac{G_s d_e}{\mu} = \frac{u_s d_e \rho}{\mu} \quad (44)$$

The shell-side heat-transfer coefficient  $h_s$  :

$$Nu = \frac{h_s d_e}{k_f} = j_h Re Pr^{0.33} \left( \frac{\mu}{\mu_w} \right)^{0.14} \quad (45)$$

The shell-side pressure drop  $\Delta P_s$  :

$$\Delta P_s = 8 j_f \left( \frac{D_s}{d_e} \right) \left( \frac{L}{l_B} \right) \left( \frac{\rho u_s^2}{2} \right) \left( \frac{\mu}{\mu_w} \right)^{-0.14} \quad (46)$$

where,  $L$  = tube length

$l_B$  = baffle spacing.

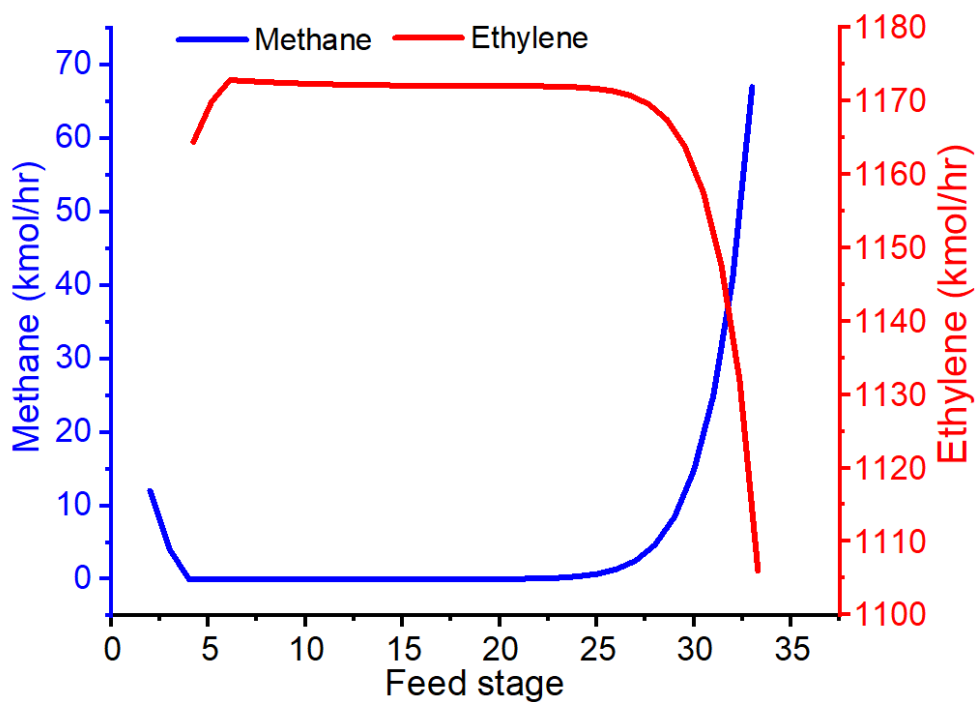
**Table D9.** Hand-calculated and Aspen Plus-derived properties of E-105

| Variable, Unit                     | Calculated | Aspen    |
|------------------------------------|------------|----------|
| Heat Duty, kW                      | 2.99E+06   | 3.15E+06 |
| LMTD, °C                           | 26.13      | 23.40    |
| Heat Transfer Area, m <sup>2</sup> | 458.15     | 487.00   |
| Assumed U, W/m <sup>2</sup> °C     | 250        | 275.704  |
| Calculated U, W/m <sup>2</sup> °C  | 295.01     |          |
| $h_i$ tube, W/m <sup>2</sup> °C    | 423.01     | 404.31   |
| $h_s$ shell, W/m <sup>2</sup> °C   | 3,169.60   | 1,913.85 |
| $\Delta P_{\text{tube}}$ , bar     | 0.02       | 0.02     |
| $\Delta P_{\text{shell}}$ , bar    | 0.00       | 0.03     |
| Velocity in a tube, m/s            | 9.46       | 12.4     |
| Velocity in a shell, m/s           | 0.57       | 0.18     |

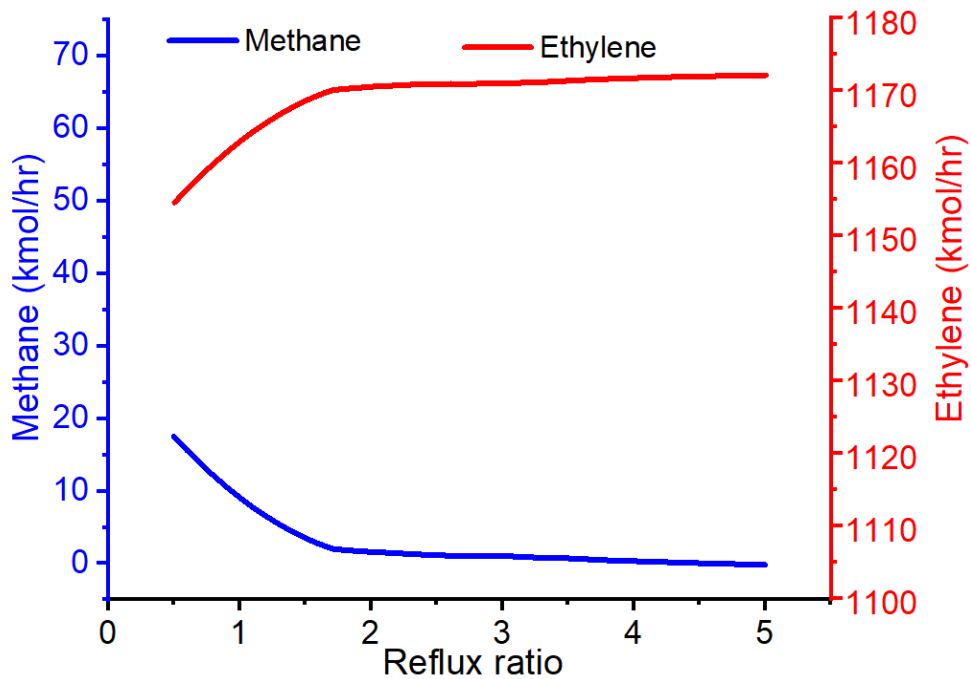
**Table D10.** Hand-calculated and Aspen Plus-derived properties of E-110

| Variable, Unit                            | Calculated | Aspen    |
|-------------------------------------------|------------|----------|
| Heat Duty, kW                             | 1.50E+06   | 1.47E+06 |
| LMTD, °C                                  | 59.13      | 58.71    |
| Heat Transfer Area, m <sup>2</sup>        | 61.24      | 58.57    |
| Assumed U, W/m <sup>2</sup> °C            | 413.00     | 427.48   |
| Calculated U, W/m <sup>2</sup> °C         | 416.10     |          |
| h <sub>i</sub> tube, W/m <sup>2</sup> °C  | 699.63     | 647.49   |
| h <sub>s</sub> shell, W/m <sup>2</sup> °C | 3458.83    | 3549.60  |
| $\Delta P_{\text{tube}}$ , bar            | 0.03       | 0.10     |
| $\Delta P_{\text{shell}}$ , bar           | 0.01       | 0.04     |
| Velocity in a tube, m/s                   | 7.10       | 9.94     |
| Velocity in a shell, m/s                  | 0.41       | 0.86     |

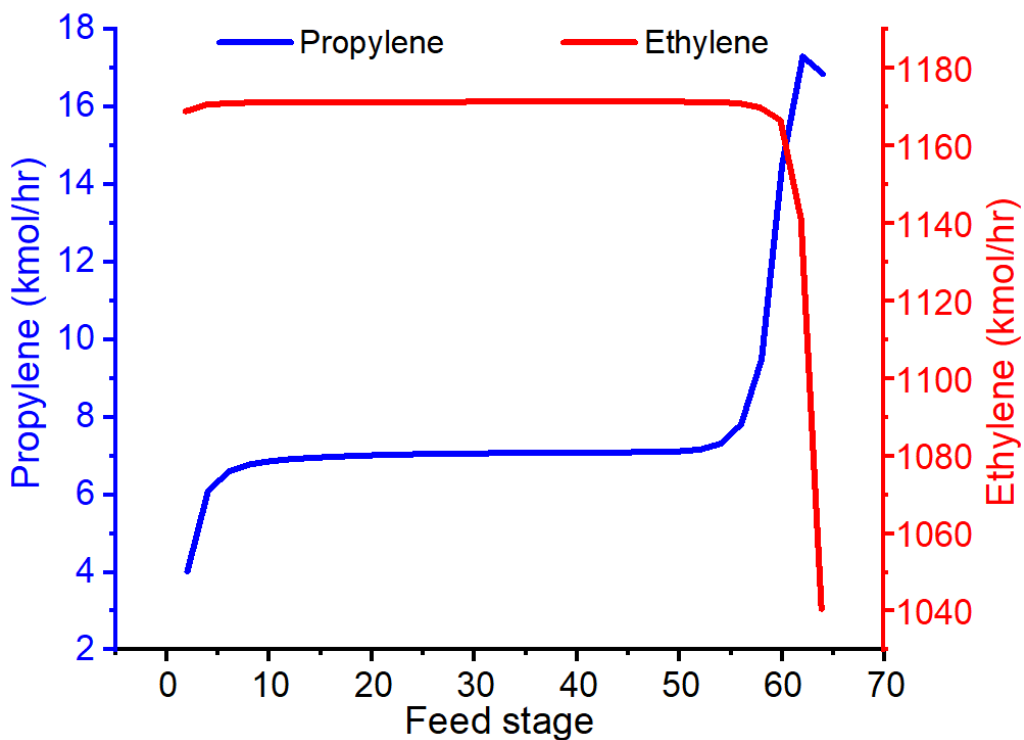
## Appendix E - Process Sensitivity Analysis and Optimization of Distillation Columns



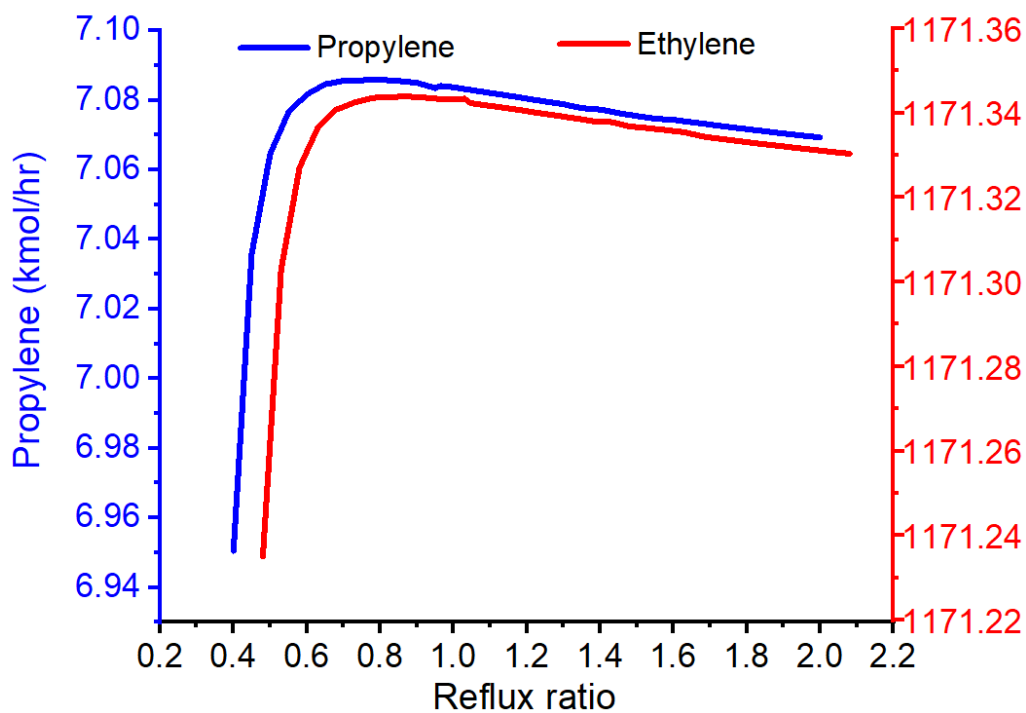
**Figure E1.** Feed stages versus methane and ethylene flowrates



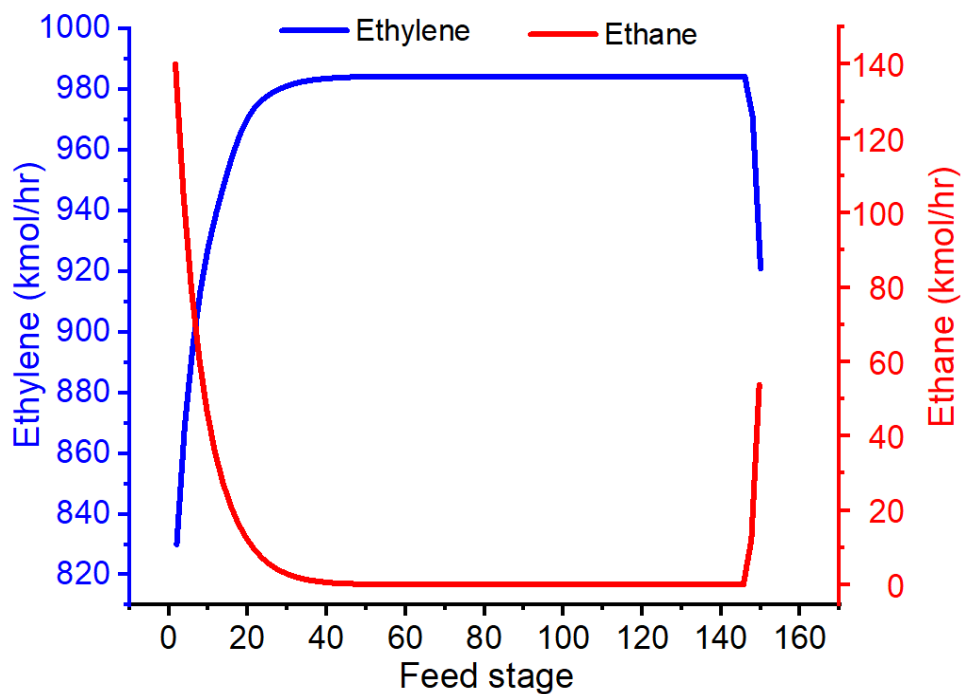
**Figure E2.** Reflux ratio versus methane and ethylene flowrates



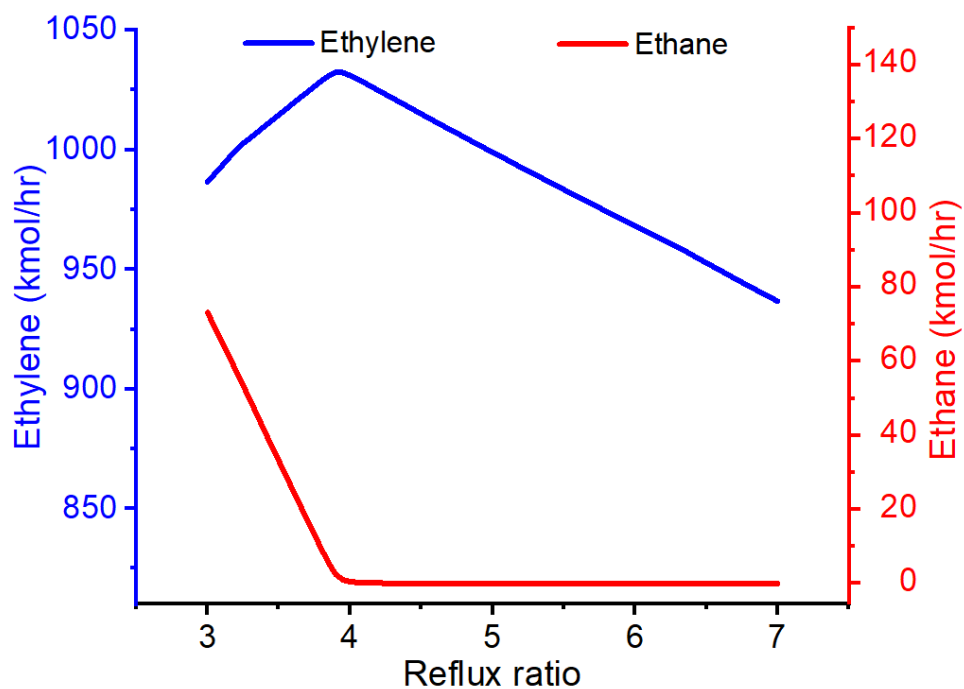
**Figure E3.** Feed stages versus propylene and ethylene flowrates



**Figure E4.** Reflux ratio versus propylene and ethylene flowrates



**Figure E5.** Feed stages versus ethylene and ethane flowrates



**Figure E6.** Reflux ratio versus ethylene and ethane flowrates

## Appendix F - Safety Assessment and NFPA Hazard Classification

**Table F1. NFPA Ethylene [10]**

| Diamond                                                                           | Hazard       | Value | Description                                                                        |
|-----------------------------------------------------------------------------------|--------------|-------|------------------------------------------------------------------------------------|
|  | Health       | 2     | Can cause short-term harm.                                                         |
|                                                                                   | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions.                       |
|                                                                                   | Instability  | 2     | Readily undergoes violent chemical changes at elevated temperatures and pressures. |

**Table F2. NFPA Ethane[10]**

| Diamond                                                                            | Hazard       | Value | Description                                                  |
|------------------------------------------------------------------------------------|--------------|-------|--------------------------------------------------------------|
|  | Health       | 1     | May cause strong irritation.                                 |
|                                                                                    | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions. |
|                                                                                    | Instability  | 0     | Stable                                                       |

**Table F3. NFPA Methane[10]**

| Diamond | Hazard       | Value | Description                                                  |
|---------|--------------|-------|--------------------------------------------------------------|
|         | Health       | 2     | Can cause short-term harm.                                   |
|         | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions. |
|         | Instability  | 0     | Stable                                                       |

**Table F4. NFPA Propane[10]**

| Diamond | Hazard       | Value | Description                                                  |
|---------|--------------|-------|--------------------------------------------------------------|
|         | Health       | 2     | Can cause short-term harm.                                   |
|         | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions. |
|         | Instability  | 0     | Stable                                                       |

**Table F5. NFPA Propylene[10]**

| Diamond | Hazard       | Value | Description                                                       |
|---------|--------------|-------|-------------------------------------------------------------------|
|         | Health       | 1     | May cause strong irritation.                                      |
|         | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions.      |
|         | Instability  | 1     | Usually stable, but unstable under high temperature and pressure. |

**Table F6. NFPA Hydrogen[10]**

| Diamond                                                                           | Hazard       | Value | Description                                                  |
|-----------------------------------------------------------------------------------|--------------|-------|--------------------------------------------------------------|
|  | Health       | 0     | No hazard                                                    |
|                                                                                   | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions. |
|                                                                                   | Instability  | 0     | Stable                                                       |

**Table F7. NFPA Acetylene[10]**

| Diamond                                                                            | Hazard       | Value | Description                                                  |
|------------------------------------------------------------------------------------|--------------|-------|--------------------------------------------------------------|
|  | Health       | 0     | No hazard                                                    |
|                                                                                    | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions. |
|                                                                                    | Instability  | 3     | Requires strong initiation or confinement to detonate.       |

**Table F8. NFPA Butadiene[10]**

| Diamond                                                                             | Hazard       | Value | Description                                                                        |
|-------------------------------------------------------------------------------------|--------------|-------|------------------------------------------------------------------------------------|
|  | Health       | 2     | Can cause short-term harm.                                                         |
|                                                                                     | Flammability | 4     | Easily flammable and quickly vaporizes at normal conditions.                       |
|                                                                                     | Instability  | 2     | Readily undergoes violent chemical changes at elevated temperatures and pressures. |

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