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Capstone Project II

Report 4

Design of Plant for Industrial Production of Ethylene in Kazakhstan

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Work distribution

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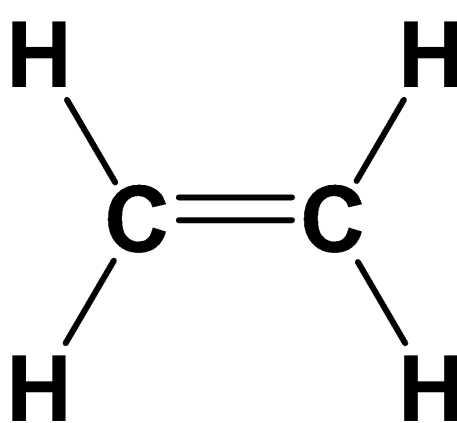
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Chapter 1. Process Introduction

1.1 Process Introduction and Rationale

Ethylene (C_2H_4) is a flammable, colourless gas with a slightly sweet odour (Table 1). It is an alkene from a simple olefin group and is primarily used as a raw material for the production of polyethylene plastic, detergents, and antifreeze. The application for ethylene arises from its presence in many chemical reactions due to the compound's high reactivity. Ethylene's reactivity stems from its structure: a planar molecule with a $C=C$ double bond that readily reacts to form polymers, hydrocarbons, or their derivatives. It occurs since electrons in π bonds are loosely held, easier to polarize than electrons in σ bonds, therefore, prone to electrophilic addition. From this follows that ethylene readily reacts with electrophilic reagents such as strong acids and halogens, but weakly with nucleophilic reagents, like bases and Grignard reagents [1].

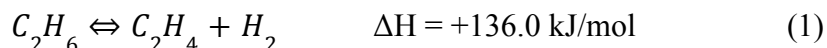
Table 1. Physical properties of ethylene.

Properties		Chemical structure
IUPAC name	Ethene	
Molecular formula	C_2H_4	
Physical appearance	Colourless gas	
Molecular mass, $g \cdot mol^{-1}$	28.0536	
Normal boiling temperature, $^{\circ}C$	-103.71	
Normal freezing temperature, $^{\circ}C$	-169.15	

Ethylene's simple structure and $C=C$ bond make it a fundamental intermediate in industrial chemistry, providing the basis for polymerization, oxidation, halogenation, and alkylation pathways of broad industrial relevance.

Steam cracking represents the predominant industrial pathway for ethylene manufacture. The method consists of two options of raw materials: naphtha and ethane. Naphtha is obtained from a fraction of crude oil, while ethane is both oil and gas. Two methods are economically feasible; however, naphtha composition is not uniform and varies significantly even over one rig. Fluctuations in paraffinic, naphthenic, and aromatic content directly affect reaction kinetics, catalyst performance, and product yield. Variation in parameters makes it difficult for design equipment and control systems to remain optimal under all feed conditions. For the following reason, plant design will be focused on ethane cracking.

The underlying process involves thermal decomposition through free radical chemistry at elevated temperatures [2].



The steam in this reactor and process is to dilute hydrocarbon partial pressures, inhibiting coke deposition, and providing thermal mass for temperature regulation. The straightforward molecular structure of ethane limits complex side reactions compared to heavier feedstocks - methane generation represents the primary competing pathway, controllable through appropriate process parameters [3].

Ethane cracking technology demonstrates remarkable commercial maturity with hundreds of operational facilities globally. Contemporary installations achieve ethane conversion of 65-70% per pass and ethylene selectivity 80-82% [4].

Numerous independent analyses validate ethane steam cracking as the most economically attractive ethylene production method. The technology exhibits economic superiority through multiple factors [5]:

The approach leverages abundant ethane resources supported by established long-duration contracts (10-20 year terms) delivering exceptional feedstock reliability. Expanding worldwide ethane availability from Middle Eastern, Russian, and other gas-rich sources ensures sustained supply security [6].

Based on the comparative evaluation of production methods, ethane steam cracking is the most technically mature and economically feasible route for ethylene production under current market conditions. Its main advantages are established infrastructure and operational experience with the reliability of technologies, feedstock availability in Kazakhstan, and lower capital expenditures.

1.2 Process Flow Diagram and Main Units Descriptions

Analyzing the existing process flows, the following diagram is proposed, depending on the composition of the feed and the required production rate of the plant. Figure 1 represents labeled stages with numbered streams, as well as their content, to make it easier to navigate and understand the diagram. It illustrates the simplified flow diagram of processes for ethylene production based on the ethane cracking method. The diagram includes a reactor, heat exchangers, mixers, compressors, and separators, which were based on the Aspen Plus modeling for heat exchangers [7].

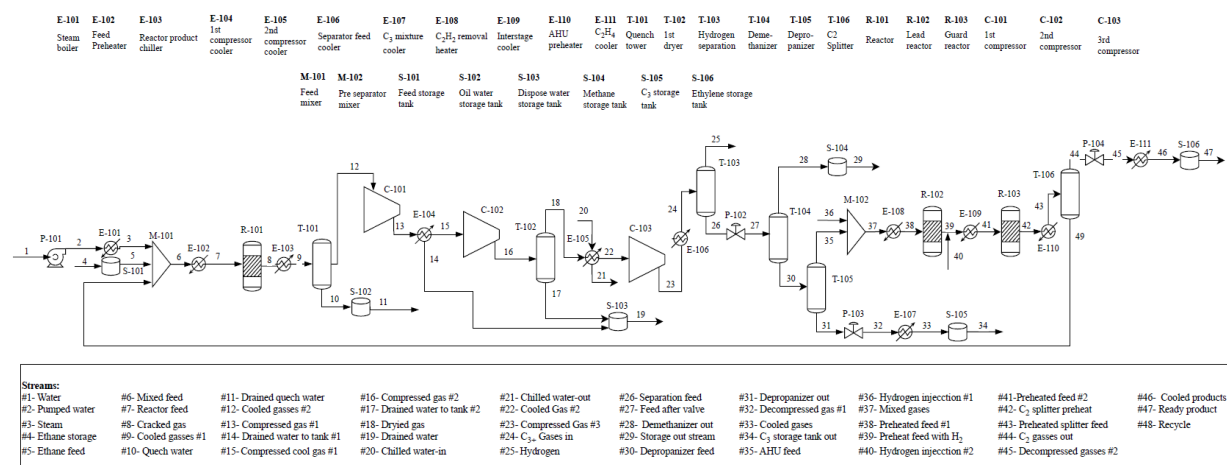


Figure 1. Steam cracking of ethane PFD

The first zone of the process is defined as the reaction zone (Table 2). It starts with the feed with water in vapor phase (Stream 1) at 107°C and 0.5 bar preheated (E-101) up to 200°C and 11 bar to enter the Feed Mixer (M-101), where the vapor phased Ethane Feed (Stream 3) is combined with a Steam (Stream 2) to form the Mixed Feed (Stream 4) [8,9,10]. The steam minimizes coking within the reactor. Following mixing, the Mixed Feed (Stream 4) is sent to the preheater (E-102), where it is brought up to 650°C temperature before entering the reactor (R-101) [11]. Within the reactor, the ethane cracking reaction is performed at a temperature of 850 °C and 2 bar with no pressure drop [12]. This process serves to convert the ethane into ethylene and byproducts. It results in the highly hot Cracked Gas product (Stream 6).

Table 2. Conditions for heaters, mixer, and reactor.

Heater	Inlet		Outlet	
	Temperature, °C	Pressure, bar	Temperature, °C	Pressure, bar
E-101	107	0.5	200	11
E-102	97.9	2.7	650	3
Mixer	Temperature, °C		Pressure, bar	
M-101	97.9		2.7	
Reactor	Temperature, °C		Pressure, bar	
R-101	850		2	
Quench	Temperature, °C		Pressure, bar	

tower		
T-101	35	2

The reactor in the Aspen Plus simulation is modeled using a Plug Flow Reactor (RPlug) block, rather than a furnace. It is because the RPlug pipes reflect the physical and chemical environment of an elongated pipe inside a real-world reactor. Therefore, it is possible to calculate the temperature, pressure, and concentration profiles along the reactor's length. There are 48 tubes with a length of 10 m and a diameter of 0.12 m [13].

To immediately stop the cracking reaction and prevent the formation of undesirable heavy end products, the hot Cracked Gas product (Stream 6) is rapidly cooled in the Quench Tower (T-101) that operates at 35°C and 2 bar pressure. The tower removes Drained Water (Stream 7) from the cooled gas stream, which gets out as Dry Gas #1 (Stream 8). Moreover, the next step requires a compression train containing 3 consecutive equipment with specifications mentioned in Table 3.

Table 3. Operating conditions for compressors and coolers.

Compressor	Inlet pressure, bar	Outlet pressure, bar
C-101	2.00	11.95
C-102	11.95	20.00
C-103	20.00	32.00
Cooler	Temperature, °C	Pressure, bar
E-103	35	11.95
E-104	35	20

Dry gases (Stream 8) leave the quench tower and call for compression before entering the dryer. Usual LPG pyrolysis systems have 3-5 compression stages, for balancing discharge temperature and meeting the required discharge pressure [14]. Furthermore, the first 2 stages of the compression have subsequent coolers to decrease the temperature of the cracked gases and remove condensed water step by step. The first compressor increases the pressure up to 11.95 bar, up to 80% of water condensed. Compressors of the second and third stages raise the pressure to 20 and 32 bar, respectively, and prepare cracked gases for drying and separation units [15].

Compressed gases (Stream 15) had eliminated most of the moisture content, but not 100%. In the case of ethylene production, separations occur at low temperatures in the range of

-13°C down to -100°C, which possibly forms hydrates and ice in the system. To prevent such scenarios, Stream 15 is passing through the dryer (T-102), where the molar fraction of water allowed into the dry spec is $1 \cdot 10^{-6}$ [16]. Such precise drying is possible using molecular sieves and chilling the feed or using glycol solutions. As a result, almost 100% of all moisture is separated at that stage [17].

The dry spec stream is directed to the fractionation train (Table 4), consisting of a hydrogen separator (T-103) first. The values for the split fractions are taken from the ethylene production simulation in Aspen Plus and the paper it was based on [18]. There, the gas feed is separated to remove mostly methane (0.9984 split fraction) and H₂ (0.9999 split fraction) as overhead products (Stream 18). The rest of the composition (Stream 19) is directed to the depropanizer (T-104), where 97.9% of propylene and 99.9% of propane are removed as bottom products (Stream 20) according to the split fraction. The overhead stream (Stream 21), containing mainly the C₂ components, is directed to the deethanizer (T-105) that separates the acetylene from ethane and ethylene. It happens in a distillation column that operates at a pressure of 18 bars, which removes trace acetylene at the bottom as purge (Stream 23) [19]. Usually, acetylene is unstable at higher pressures. However, due to its low mass fraction compared to other components, the pressure is kept between the depropanizer and C₂-splitter in accordance with the Aspen model, which might not be industrially accurate. The top stream (Stream 22) of the deethanizer is headed to the C₂-splitter (T-106) that operates at 16.56 bar and separates ethylene product at 99.9% purity (0.999 split fraction) as an overhead stream (Stream 24), and the ethane stream (Stream 25) is recycled back to the feed mixer (M-101) [20].

Table 4. Operating conditions for separators.

Unit	Feed temperature, °C	Pressure, bar
T-103	77.7	35.15
T-104	5.5	23.44
T-105	-13.7	18
T-106	-24.6	16.56

Chapter 2. Process Summary

The total production rate of ethylene is 300000 t/year. With a planned operation schedule of 7632 hours (or 318 days), the production rate is equivalent to 786.16 t/day or 32.75 t/h (32,757 kg/hr). The feed stream (Table 5) consists of a hydrocarbon-rich mixture with a total mass flow rate of 39000 kg/hr, corresponding to approximately 1295.29 kmol/h molar flow rate. The stream's average molecular weight is 30.11 kg/kmol. Ethane is the primary component of the feed stream, representing 94.00% by weight with a flow rate of 34415.24 kg/hr or 1217.57 kmol/hr. Propane represents the second most significant component at 3.00% by weight, contributing 51.41 kg/hr or 38.86 kmol/h to the total flow. Methane, the lightest hydrocarbon present in the stream, accounts for 1.00% by weight with a flow rate of 2.08 kg/hr or 12.95 kmol/hr.

Table 5. The molar flow rate for Feed, Water, Recycle, and Mixture.

Operating Conditions	1	2	3	4	5	6
Temperature, °C	25	25	200	20	73	650
Pressure, bar	1	11	11	1	1	2
Vapor fraction	0	0	1	1	0.91	1
Initial Feed						
Compound\Stream, kmol/hr	1	2	3	4	5	6
C ₂ H ₆	0	0	0	1217.57	1919.31	1919.31
C ₃ H ₈	0	0	0	38.86	38.89	38.89
C ₂ H ₄	0	0	0	0	21.90	21.90
H ₂	0	0	0	0	0	0
CH ₄	0	0	0	12.95	12.95	12.95
C ₂ H ₂	0	0	0	0	0.04	0.04
H ₂ O	1110.17	1110.17	1110.17	25.91	1136.07	1136.07
C ₃ H ₆	0	0	0	0	0.45	0.45
Total	1110.17	1110.17	1110.17	1295.29	3129.62	3129.62

The thermal cracking reactor operates at 1123.15 K (850°C) with a space time of 0.1079 seconds, and it has four reactions.

$$X_{C_2H_6} = 1 - e^{-k_1\tau} \Rightarrow \tau = -\frac{\ln(1-X_{C_2H_6})}{k_1} = -\frac{\ln(1-0.6431)}{9.5499} \approx 0.1079 \text{ s} \quad (2)$$

The reactor achieves 83.10% overall ethane conversion, with the primary dehydrogenation route contributing 73.34% conversion. Ethylene selectivity reaches 98.8% with respect to combined R1 and R3 pathways. The product distribution for validation and recycle cases shows ethylene production of 1869.84 and 1880.82 kmol/hr, respectively, hydrogen production exceeding 900 kmol/hr, methane formation of 1230.69 and 1271.33 kmol/hr, unconverted ethane of 38.86 kmol/h, and acetylene formation of 12.54 and 12.96 kmol/hr. The reaction extents for validation and recycle cases are 892.93 and 1,215.42 kmol/hr for R1, 15.47 and 13.96 kmol/hr for R2, 16.82 and 15.18 kmol/hr for R3, and 1.37 and 0.93 kmol/hr for R4. The substantial methane formation, increasing from approximately 13 kmol/hr in the feed to over 1,230 kmol/hr in the product, represents significant carbon loss primarily from propane cracking. Hydrogen production exceeding 900 kmol/hr can be recovered as a valuable byproduct for use in hydrogenation processes, refinery operations, or hydrogen energy applications. Acetylene formation, while modest at 12.5-13.0 kmol/hr, requires downstream hydrogenation or separation as it poisons polymerization catalysts.

The 12.3% difference between validation (83.10% conversion) and recycle (74.99% conversion) cases indicates that recycle stream composition significantly impacts reactor performance (Table 6). Accumulation of hydrogen, methane, and other light components in the recycle loop reduces partial pressures of reactive species, affecting reaction rates and equilibrium positions.

Table 6. Molar flow rate for the reactor inlet and outlet streams.

Operating Conditions	7	8
Temperature, °C	650	850
Pressure, bar	2	2
Vapor fraction	1	1
Reactor		
Compound\Stream, kmol/hr	7	8
C ₂ H ₆	1919.31	700.21
C ₃ H ₈	38.89	7.58
C ₂ H ₄	21.90	1257.29
H ₂	0	1234.12
CH ₄	12.95	30.40
C ₂ H ₂	0.04	1.20
H ₂ O	1136.07	1136.07
C ₃ H ₆	0.45	14.31
Total	3129.62	4381.18

Molar selectivity:

$$S_{total} = \frac{\text{Moles Ethylene Produced}}{\text{Moles Ethane and Propane Consumed}} * 100 = \frac{1230.60}{1215.42+29.19} * 100 = 98.88\% \quad (3)$$

Mass selectivity:

$$S_{mass} = \frac{1230.6*28.05}{1215.42*30.07} * 100 = 94.45\% \quad (4)$$

According to Table 7, reacted gases then headed to the quench tower (T-101) to decrease the temperature from 850°C to 35°C and separate more than 90% portion of the water before the compressors train to prevent equipment damage. As a result, the stream leaving the quench tower contains 1056.3221 kmol/hr of water, and Stream 8 heading to the compressors contains around 2.5% water. Stream 8 enters the first stage compressor (C-101) at a pressure of 2 bars and 35°C and leaves at 202.01°C, and 11.95 bars. The resulting exit stream has the same composition and passes through the dryer to remove water and then goes to the cooler E-105 to cool the feed. Cooler E-104 removes 62.58 kmol/hr of water, and the stream moves to a second-stage compressor.

Table 7. Reactor product and quench tower streams

Operating Conditions	9	10	11	12	13
Temperature, °C	350	35	35	35	201
Pressure, bar	2	2	2	2	11.95
Vapor fraction	1	0	0	0	1
Before separation					
Compound/ Stream, kmol/hr	9	10	11	12	13
C ₂ H ₆	700.21	0	0	700.21	700.21
C ₃ H ₈	7.58	0	0	7.58	7.58
C ₂ H ₄	1257.29	0	0	1257.29	1257.29
H ₂	1234.12	0	0	1234.12	1234.12
CH ₄	30.40	0	0	30.40	30.40
C ₂ H ₂	1.20	0	0	1.2	1.2
H ₂ O	1136.07	1056.04	1056.04	80.04	80.04
C ₃ H ₆	14.31	0	0	14.31	14.31
Total	4381.18	1056.04	1056.04	3325.15	3325.15

The second stage compressor at the Table 8 (C-102) results in a compressor stream that has 20 bar pressure and 81.66°C. Compressed Stream 12 goes through a dryer (T-102) that

removes 17.45 kmol/hr of water. Then enters the heat exchanger (E-105) and decreases the temperature to 35°C and, leaving almost no water. The next stream from Table 9 coming from the cooler moves to the final stage compressor (C-103), where gases are compressed to the target 32 bars required for separation units at the ethylene plant. However, cracked gases should be dehydrogenated too, before separation to prevent fouling of separator, as the temperature inside separators decreases down to -100°C, so stream leaving the compressor station should pass through a hydrogen separation (T-103) that removes 100% of H₂ from the stream.

Table 8. 2nd stage compressor, dryer and heat exchanger streams

Operating Conditions	14	15	16	17	18
Temperature, °C	35	35	82	82	82
Pressure, bar	11.95	11.95	20	20	20
Vapor fraction	0	1	1	0	1
Before separation					
Compound\ Stream, kmol/hr	14	15	16	17	18
C ₂ H ₆	0	700.21	700.21	0	700.21
C ₃ H ₈	0	7.58	7.58	0	7.58
C ₂ H ₄	0	1257.29	1257.29	0	1257.29
H ₂	0	1234.12	1234.12	0	1234.12
CH ₄	0	30.40	30.40	0	30.40
C ₂ H ₂	0	1.2	1.2	0	1.2
H ₂ O	62.58	17.45	17.45	17.45	0
C ₃ H ₆	0	14.31	14.31	0	14.31
Total	3212.82	3262.57	3262.57	17.45	3245.11

Table 9. 3rd stage compressor and separation feed streams

Operating Conditions	19	20	21	22	23	24	25
Temperature, °C	63	20	35	31	81	-104	-104
Pressure, bar	12	5	5	20	35	35	35
Vapor fraction	0	0	0	1	1	0.39	1
Separation							
Compound\ Stream, kmol/hr	19	20	21	22	23	24	25

Stream, kmol/hr							
C ₂ H ₆	0	0	0	700.21	700.21	700.21	0
C ₃ H ₈	0	0	0	7.58	7.58	7.58	0
C ₂ H ₄	0	0	0	1257.29	1257.29	1257.29	0
H ₂	0	0	0	1234.12	1234.12	1234.12	1209.43
CH ₄	0	0	0	30.40	30.40	30.40	0
C ₂ H ₂	0	0	0	1.2	1.2	1.2	0
H ₂ O	80.04	6000.91	6000.91	0	0	0	0
C ₃ H ₆	0	0	0	14.31	14.31	14.31	0
Total	80.04	6000.91	1926.22	3245.11	3245.11	3245.11	1209.43

The stream 27 from Table 10 enters the demethanizer at a temperature of -104°C and at 35 bar. There, the column separates the dried gas into an overhead stream that contains mainly H₂ and CH₄. The stream is connected to the depropanizer (T-105), where at 31 bar, C₃ products, propane, and propylene are removed with stream 31. This leads to top stream 35 (Table 12), mostly containing ethane, ethylene and acetylene that needs to be separated. In the acetylene hydrogenation unit, 99.9% of the acetylene is removed through the reaction hydrogenation (Table 13). Thus, C2-splitter (T-106) is a separate product of acetylene hydrogenation unit, as ethane and we receive purified ethylene as a main product (Table 14).

As shown in Table 15, around 1231.8 kmol/hr (Aspen) of ethylene is separated as a final product in stream at -104°C and 1 bar. The split down ethane (701.74 kmol/hr in Aspen) is accumulated in stream at -19 °C and recycled back to the Feed Mixer.

Table 10. Demethanizer feed and product streams

Operating Conditions	26	27	28	29
Temperature, °C	-104	-104	-101	-101
Pressure, bar	35	35	30	30
Vapor fraction	0	0	1	1
Ethylene Separation				
Compound\ Stream, kmol/hr	26	27	28	29
C ₂ H ₆	700.21	700.21	0.14	0.14
C ₃ H ₈	7.58	7.58	0	0
C ₂ H ₄	1257.29	1257.29	1.77	1.77
H ₂	24.68	24.68	24.68	24.68

CH ₄	30.40	30.40	30.40	30.40
C ₂ H ₂	1.20	1.20	0	0
H ₂ O	0	0	0	0
C ₃ H ₆	14.31	14.31	0	0
Total	2035.67	2035.67	57.00	57.00

Table 11. Depropanizer streams

Operating Conditions	30	31	32	33
Temperature, °C	-4	71	-46	-47
Pressure, bar	31	30	1	1
Vapor fraction	0	0	0.74	0
Separation				
Compound\ Stream, kmol/hr	30	31	32	33
C ₂ H ₆	700.07	0.07	0.07	0.07
C ₃ H ₈	7.577	7.55	7.55	7.55
C ₂ H ₄	1255.52	0	0	0
H ₂	0	0	0	0
CH ₄	0	0	0	0
C ₂ H ₂	1.20	0	0	0
H ₂ O	0	0	0	0
C ₃ H ₆	14.31	13.86	13.86	13.86
Total	3206.76	21.48	21.48	21.48

Table 12. Depropanizer product and Acetylene hydrogenation unit feed

Operating Conditions	34	35	36	37
Temperature, °C	-47	-5	25	-15
Pressure, bar	1	30	25	25
Vapor fraction	0	1	1	1
Separation				
Compound\ Stream, kmol/hr	34	35	36	37

C ₂ H ₆	0.07	700	0	700
C ₃ H ₈	7.55	0.03	0	0.03
C ₂ H ₄	0	1255.51	0	1255.51
H ₂	0	0	3.31	3.31
CH ₄	0	0	0	0
C ₂ H ₂	0	1.20	0	1.20
H ₂ O	0	0	0	0
C ₃ H ₆	13.86	0.45	0	0.45
Total	21.48	1957.19	3.31	1960.5

Table 13. Acetylene hydrogenation unit streams

Operating Conditions	38	39	40	41
Temperature, °C	60	63	50	60
Pressure, bar	25	25	25	25
Vapor fraction	1	1	1	1
Separation				
Compound\ Stream, kmol/hr	38	39	40	41
C ₂ H ₆	700	701.69	0	701.69
C ₃ H ₈	0.03	0.03	0	0.03
C ₂ H ₄	1255.51	1254.45	0	1254.45
H ₂	3.31	0.98	0.65	1.6314
CH ₄	0	0	0	0
C ₂ H ₂	1.20	0.57	0	0.57
H ₂ O	0	0	0	0
C ₃ H ₆	0.45	0.45	0	0.45
Total	1960.5	1958.17	0.65	1958.82

Table 14. C₂ splitter feed and product

Operating Conditions	42	43	44	45
Temperature, °C	62	-40	-41	-103
Pressure, bar	25	15	14	1
Vapor fraction	1	0	0	0.33

Separation				
Compound\ Stream, kmol/hr	42	43	44	45
C ₂ H ₆	702.69	702.69	1.16	1.16
C ₃ H ₈	0.03	0.03	0	0
C ₂ H ₄	1253.7	1253.7	1231.8	1231.8
H ₂	0	0	0	0
CH ₄	0	0	0	0
C ₂ H ₂	0.11	0.11	0.07	0.07
H ₂ O	0	0	0	0
C ₃ H ₆	0.45	0.45	0	0
Total	1957.19	1957.19	1233.03	1233.03

Table 15. Product and Recycle streams

Operating Conditions	46	47	48
Temperature, °C	-104	-104	-19
Pressure, bar	1	1	15
Vapor fraction	0	0	0
Separation			
Compound\ Stream, kmol/hr	46	47	48
C ₂ H ₆	1.16	1.16	701.74
C ₃ H ₈	0	0	0.03
C ₂ H ₄	1231.8	1231.8	21.9
H ₂	0	0	0
CH ₄	0	0	0
C ₂ H ₂	0.07	0.07	0.05
H ₂ O	0	0	0
C ₃ H ₆	0	0	0.45
Total	1233.03	1233.03	724.161

Chapter 3. Major Equipment Design

3.1 R-101 Cracking Furnace Reactor

Process Description

For the ethylene production plant, the main reactor is the cracking furnace reactor. Steam ethane cracking is carried out in long vertical tubular reactors, also known as radiant coils, which are suspended in a gas-fired furnace box. The process gas enters the radiant coils at 650 °C and is heated to 850 °C; for design calculations, an isothermal operation at 850 °C was assumed along the length of the tube.

The reaction is a highly endothermic non-catalytic reaction; it requires huge amounts of energy to break both C-C (345 kJ/mole) and C-H (413 kJ/mole) bonds [22]. Although the reaction itself is not catalytic, the reactor materials themselves, nickel and iron, can act as a catalyst for the coke formation. A carbon-rich atmosphere in direct contact with metals induces the hydrocarbons to be chemisorbed on the catalytic sites, subsequently losing hydrogen and leaving carbon deposits on the walls of the reactor [22]. Steam is added as an inert diluent to decrease the partial pressure of hydrocarbons to mitigate the coke formation problem. The Steam-to-Hydrocarbon (S/HC) weight ratio ranges between 0.3 and 0.5 [23].

Typical conditions for this process are in the range of 800 to 950°C, and 1-5 bars. Short residence time is usually taken to be 0.1-0.8 seconds, to prevent further side reactions [24]. The key design parameters selected for R-101 are 850°C, 2 bar, and a residence time of approximately 0.13-0.16 s.

Reaction Network and Kinetics

To model the cracking process, the network of 4 reactions was selected and validated in Report 2. The model consists of primary ethane dehydrogenation (R8), propane cracking side reactions (R1, R2), and a propylene cracking secondary reaction (R6). For the reversible reactions R6 and R8, rate constants for reverse reactions were calculated from equilibrium data to implement them into Aspen Plus as a power law type reaction; the derivations are presented in an Excel file. Table A1 in Appendix A summarizes all the reactions. The kinetic model and rate expressions were developed and validated in Report 2.

Reactor Design Methodology

A Plug Flow Reactor (PFR) is widely used for this process because it gives the highest conversion per unit volume for positive order reactions. To account for reasonable pressure drop and fluid velocity, R-101 was designed as a multi-tube fired PFR, with gas flowing upward through vertical tubes.

Steady state equations were used to calculate the reactor volume, the Euler Method to solve the system of ODEs, and the Haaland equation for pressure drop [25]. The hand-calculated values match the Aspen Plus simulation.

The 77 tubes are arranged vertically inside the furnace in a configuration similar to the shell-and-tube heat exchanger. Assuming a tube pitch of $1.5 \times D_o$, the upper bound of the standard TEMA range is 1.25–1.5 [26]. The centre-to-centre distance between tubes is approximately 250 mm. Considering a 7×11 configuration, the preliminary size of the tube bundle is 1.75×2.75 m, which should be adjusted further based on the heat duty of 65657 kW obtained directly from the Aspen Plus simulation. The height is determined by the tube length and clearance for the floor/ceiling and inlet/outlet headers. The corresponding calculation methodology in Appendix B and material selection is described in Appendix C in detail. The summarized reactor design can be seen in Table 11. The arrangement of tubes in one layer of the reactor is shown in Figure 2.

Table 16. Reactor Design Summary.

Parameter	Value		Parameter	Value	
Reactor type	Fired Tubular PFR, multi-tubed		Required Wall Thickness	2.46 mm	
Operating Temperature	850°C		Tube Length	4.57 m	15 feet
Operating pressure	2 bar		Tube Arrangement	7x11 grid	
Ethane conversion	63.92%		Tube Bundle Sizes	1.75x2.75 m	
Heat duty	65,66 kW		Reactor Height	6.57 m	
Residence time	Handcalc.	Aspen Plus	Inlet Gas Velocity	15.33 m/s	
	0.165 s	0.130 s	Outlet Gas Velocity	39.31 m/s	
S/HC ratio	0.35		Pressure drop	0.0016 bar	
Total reactor volume	6.5 m ³		Tube Material	HP40-Nb centrifugal cast alloy	
Number of tubes	77		Design Lifetime	5 years	
Tube schedule (ASME)	Schedule 40, 6-inch nominal		Nominal wall thickness	7.112 mm	0.280 in
Tube outside diameter	168.275 mm	6.625 in	Tube inside diameter	154.051 mm	6.065 in

Sensitivity analysis in Aspen Plus was done, varying the length of the reactor without pressure drop with an inner diameter of 0.15405 m. The needed conversion is reached at around 350 m, while increasing the reactor twice in length increases the conversion just by 10%, meaning that further increase in reactor volume is not feasible. The sensitivity results are shown in Figure 3.

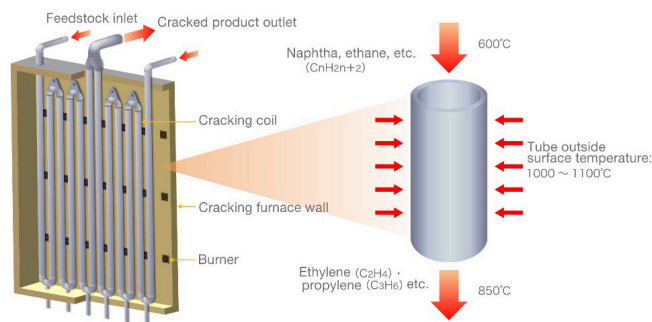


Figure 2. Layout of one layer of the reactor [27].

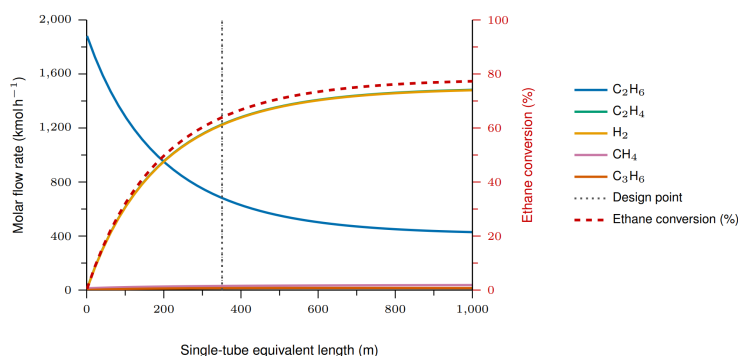


Figure 3. Sensitivity analysis of the product flow rates vs. reactor length.

3.2 E-104 Heat Exchanger Design

Design Basis and Process Conditions

Heat exchangers are an essential part of the industrial plants' thermal systems. The primary goal of heat exchangers is to transfer heat efficiently between various media. Heat transfer principles and equations are the fundamentals for designing efficient and feasible heat exchangers. Ethylene plants have various stream conditions to operate, as a result, there could be all types of heat exchangers, such as shell and tube, plate, or air-cooled. This section focuses on these principles to produce a heat exchanger design.

E-104 interstage cooler is designed for the ethylene plant compression station, where the feed temperature rises after the compression and should be decreased before entering the next compressor. This is required to avoid operational issues, such as improving thermodynamic efficiency by reducing the specific work of compression in the subsequent stage, as well as

protecting compressor mechanical components, such as seals and valves, from excessive discharge temperatures. Diolefin polymerization and water condensation are secondary concerns managed through inhibitor injection and residence time control [28]. Our plant compression station operates in 3 progressive stages to increase pressure step by step. The first step starts at 2 bar to 11.9 bar, and subsequent 20 and 30 bar compression with interstage coolers between the compression equipment. Equipment designed in this section is the cooler located between the second and third compressor stages, and its function is to reduce the temperature of the feed from 81.66°C at the inlet to 30°C at the outlet. The design requirements were taken from the Capstone II Aspen Plus model, with several modifications for feasibility. All necessary data for calculations are in Table 2.

E-104 is designed as a shell-and-tube heat exchanger for high-pressure service and provides a robust configuration for both operation and maintenance. The selected parameters are one shell pass and four tube passes, with hot feed gas in the shell and cooling water at the tube side. As the temperature for cooling is the water working range, it was decided to use cooling tower water from 20°C to 30°C. It was decided to put cooling water into tubes to prevent pressure drop and to ensure easy cleaning and maintenance. The selected material is SS316L, as it is suitable for use with water and the selected feed of light hydrocarbon gases. This alloy suits our medium and high-temperature/pressure processes. Moreover, corrosion resistance and longevity, with cheap costs, make SS316L a feasible material for E-104 [29].

Thermal and Hydraulic Design

Design methodologies required for heat exchangers do not follow one set of straight instructions, but rather a workflow that combines thermal sizing, hydraulic changes, and mechanical specifications. In general, heat transfer equipment can be sized using the LMTD method when inlet and outlet temperatures are known or the ϵ -NTU method when the outlet temperature is unknown, and effectiveness is more important. Our calculations followed the LMTD method and rating approach as all four terminal temperatures were defined, allowing direct calculation of the mean temperature driving force without iteration. The selected methodology uses an energy balance to calculate the duty, followed by LMTD area sizing with an appropriate correction factor, and then verification using pressure drop in the tube and shell. Aspen Plus is used as a verification tool to confirm that the final geometry is feasible and meets the duty and pressure-drop requirements.

Several iterations were made to make both heat-transfer performance and a mechanically feasible design. An initial design idea was to use a six-tube pass with triangular tube placement with a single-segmental baffle type. However, the calculation of pressure drop and velocity showed unacceptable velocity of the gas in the shell side. Moreover, it caused vibration issues in the Aspen Plus simulation. Then it was decided to move to a rod baffle type that adds more stability for the heat exchanger's tubes. The advantages of the rod baffle type, except for solving the vibrations issue, were better flow dynamics that make heat transfer more effective, lower

pressure drop across the shell side, and reduced susceptibility to flow-induced tube vibration [30]. Moreover, the baffle spacing was significantly reduced compared to the segmental baffle type, from 0.8D to 0.23D, for the rod baffles. An additional process complication parameter was the velocity of the cooling water inside the tube. The tube passes, and the length was chosen to maintain the necessary velocity to prevent flow stagnation and fouling deposit accumulation and, at the same time, control vibration.

The next issue the design faced was the condensation of water contained in the feed, which made the whole process more complex, as it involved two-phase behaviour and latent heat effects. To keep the design consistent with previous reports, it was decided to add a dryer after the compression to reduce water content, allowing calculations for E-104 to be without condensation inside the shell. Under this assumption, the rod-baffle design was completed and validated in Aspen Plus V14.

Simulation Validation and Final Equipment Specification

Table 17 summarizes the thermal and physical properties of the hot and cold fluid streams used in the heat exchanger design.

Table 17. Values for the calculation basis.

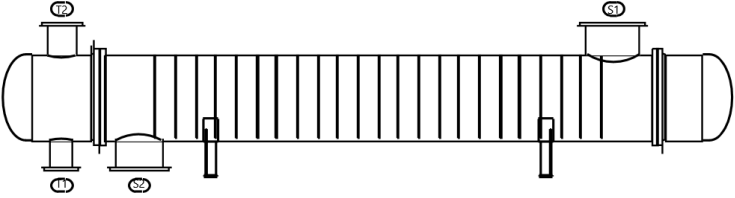
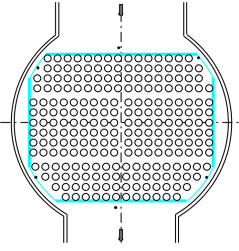
Parameter	Hot fluid (Shell-side)	Cold Fluid (Tube-side)
Inlet temperature, °C	82	20
Outlet temperature, °C	30	30
Mass flow rate, kg/h	61382.6	-
Mass flow rate, kg/s	17.1	47
Thermal conductivity, W/(m·K)	0.055	0.615
Viscosity, Pa·s	1.412E-5	0.001
Heat capacity, kJ/(kg·K)	2.454	4.178
Density, kg/m ³	12.6	997

Comparison of hand calculations and Aspen simulation was made for Area and Heat Duty in Table 18. Close values of these parameters provide confidence that thermal sizing calculations and methodology are properly selected for the following process. Full traceable calculations provided in the Appendix. Full specification of the unit can be found in Table 19.

Table 18. Comparison of area and heat duty of hand calculation and Aspen Plus simulation.

Parameter	Hand Calculation	Aspen Plus V14
Area, m ²	179.68	175.7
Heat Duty, kW	2173.30	2150.52

Table 19. Specification sheet for E-104.

Setting Plan		Tube Layout
		
Parameter	Tube side	Shell side
Length, m	4.2	
Inner diameter, m	0.0217	0.697
Outer diameter, m	0.025	0.719
Pitch diameter, m	0.0312	
Baffle spacing	0.162	
Baffle type	Rod	
Tube pattern	90-Square	
Number of tubes	559	
Tube passes	4	-
Shell in series	-	1
Shell in parallel	-	1
Pressure drop, bar	0.14	0.12
Type of material	SS 316L	

3.3 T-104 Demethanizer

The role of the Demethanizer

The role of the demethanizer is to split the methane component from the rest of the cracked mixture [28]. Additionally, hydrogen is removed concurrently with the overhead methane, while the other components of the cracked gas go to the bottom. The overhead product then goes to the cold box and is separated into a hydrogen-rich tail gas and a methane-rich tail gas [31]. This is done to produce hydrogen-rich gas and methane fuel. The bottoms, consisting of C_2 and heavier hydrocarbons, proceed into the downstream recovery train, including the deethanizer and C_2 splitter.

Demethanization is performed under cryogenic conditions so that methane can be separated by distillation from C_2+ components and to enable sufficient condensation for reflux. Depending on operating pressure and feed composition, overhead temperatures typically range from approximately 130–165K, while operating pressures in industrial demethanizers generally lie between 25 and 40 bar [32]. Due to the very low temperatures in the cryogenic section, it is essential to remove any traces of acid gases (CO_2) and water upstream of the column to prevent freezing and solid formation inside the unit.

The plant design in this report utilises ethylene production by steam cracking with a front-end demethanizer. This configuration was selected primarily because it reduces refrigeration load and compressor duty by removing hydrogen and methane, the lightest and most volatile components, ahead of the main fractionation train. A secondary benefit is that the downstream columns, including the deethanizer and C_2 splitter, handle a lighter-depleted feed, reducing their required size and operating duty.

The working principle

Hydrogen is practically non-condensable in cracked gas under cryogenic conditions. Only 33.2K is its critical temperature, which is significantly lower than any demethanizer's operating temperature. As a result, hydrogen leaves the column overhead and stays completely in the vapor phase. Compared to the C_2+ components, methane is significantly more volatile, even though it can condense under cryogenic conditions. Methane is enriched in the overhead product, and the C_2+ fraction is recovered in the bottoms when the column is configured correctly and there is enough reflux.

Maintaining a high column pressure is crucial for a number of important design considerations. In order to generate reflux using the available refrigeration levels without the need for a deeper, more expensive refrigerant cycle, it first raises the mixture's dew and bubble points. Second, increased pressure causes vapour density to rise, which lowers the volumetric vapour flow rate for a given molar throughput. This, along with the corresponding rise in permissible vapour velocity, lowers the necessary column diameter.

Demethanizer Design Calculations

This report presents the preliminary design of a demethanizer column for the separation of methane from an ethylene-rich hydrocarbon stream. The column operates at cryogenic conditions ($T = 169.15 \text{ K}$, $P = 35.15 \text{ bar}$) and must achieve a very sharp separation: 99.99 % of methane must be recovered overhead, while ethylene loss to the distillate is limited to 0.01 %. This purity requirement is driven by the downstream C2 splitter, where even trace methane would compromise ethylene product specification.

Methane and ethylene are designated as the light key (LK) and heavy key (HK) components, respectively. The Fenske–Underwood–Gilliland (FUG) shortcut method was employed for all stage and reflux calculations, with vapour–liquid equilibrium (VLE) K-values computed from the modified Wilson correlation [33].

Feed Characterisation and Operating Basis

The feed stream enters at a flow rate of 1961.3 kmol/hr and consists predominantly of ethylene (62.5 mol%) and ethane (34.8 mol%), with methane comprising only 1.55 mol %. Despite its low concentration, methane's complete removal is essential for final product purity.

Table 20. Operation Conditions.

Operating Conditions		
Parameter	Value	Units
Temperature	-104	°C
Pressure	35.15	bar
Temperature, K	169.15	K

The feed enters at -104°C , approximately 120K below its bubble point of -3.87°C , giving a feed quality of $q = 2.434$. A subcooled feed of this magnitude has a pronounced effect on column hydraulics: the additional sensible-heat load forces a large increase in liquid flow throughout the stripping section, which in turn demands a proportional increase in vapour flow to maintain the internal material balance. As shown in the next sections, this asymmetry is the primary driver of the unusual geometry of the column.

Vapour–Liquid Equilibrium and Relative Volatilities

K-values were calculated at the design conditions using the modified Wilson correlation [34]:

$$K = \left(\frac{P_c}{P}\right) \cdot \exp\left[C \cdot (1 + \omega) \cdot \left(1 - \frac{T_c}{T}\right)\right] \quad (5)$$

Relative volatilities were then referenced to ethylene (the heavy key). To assess sensitivity, the RadFrac method was applied, and the value of $\alpha_{LK} = 3.116$ was adopted as the basis for all

subsequent calculations. The value of C in the Wilson correlation was calibrated as 2.62 due to extreme conditions with high pressure and cryogenic temperatures.

Shortcut Design: Fenske-Underwood-Gilliland Method

At total reflux, the minimum number of equilibrium stages is given by the Fenske equation:

$$N_m = \frac{\log\left(\left(\frac{x_{LK}}{x_{HK}}\right)_D \left(\frac{x_{HK}}{x_{LK}}\right)_B\right)}{\log(\alpha_{LK})} \quad (6)$$

Substituting the specified split fractions yields $N_m = 18.0$ stages.

The Underwood root θ , which was found through numerical solution in Excel, satisfies $\alpha_{HK} < \theta < \alpha_{LK}$ ($1.0 < \theta < 2.78$) and equals 1.533. The factor $(1 - q) = -1.434$ is negative because $q = 2.434 > 1$, which causes θ to move toward lower values in comparison to a saturated-liquid feed and raises the calculated minimum reflux. The methane/ethylene separation's moderate intrinsic difficulty is reflected in the Underwood equation's relatively modest value of $R_{min} = 1.047$.

$$R_{min} = \sum_i \frac{X_{D,i} \alpha_i}{\alpha_i - \theta} - 1 = 0.9533 \quad (7)$$

$$R = 1.1 * R_{min} = 1.0486 \quad (8)$$

$R = 0.95 R_{min} = 1.05$ was the operating reflux setting. For cryogenic columns, where minimizing condenser duty is the primary economic constraint due to refrigeration costs, a ratio of $R/R_{min} = 1.1$ is standard practice.

The Eduljee explicit approximation to the Gilliland correlation relates the stage count to the reflux ratio through the dimensionless parameters [35]:

$$X = \frac{R - R_{min}}{R + 1} \quad (9)$$

$$Y = 1 - \exp\left[\left(\frac{1 + 54.4 * X}{11 + 117.2 * X}\right) * \left(\frac{X - 1}{\sqrt{X}}\right)\right] \quad (10)$$

The number of theoretical stages is:

$$N = \frac{N_{min} + Y}{1 - Y} \quad (11)$$

Assuming an overall tray efficiency 60% [36]

$$N_{actual} = \frac{N}{E} \quad (12)$$

The Gilliland correlation predicts $N_{theoretical} = 50.4$ theoretical stages, giving $N_{actual} \approx 84$ stages.

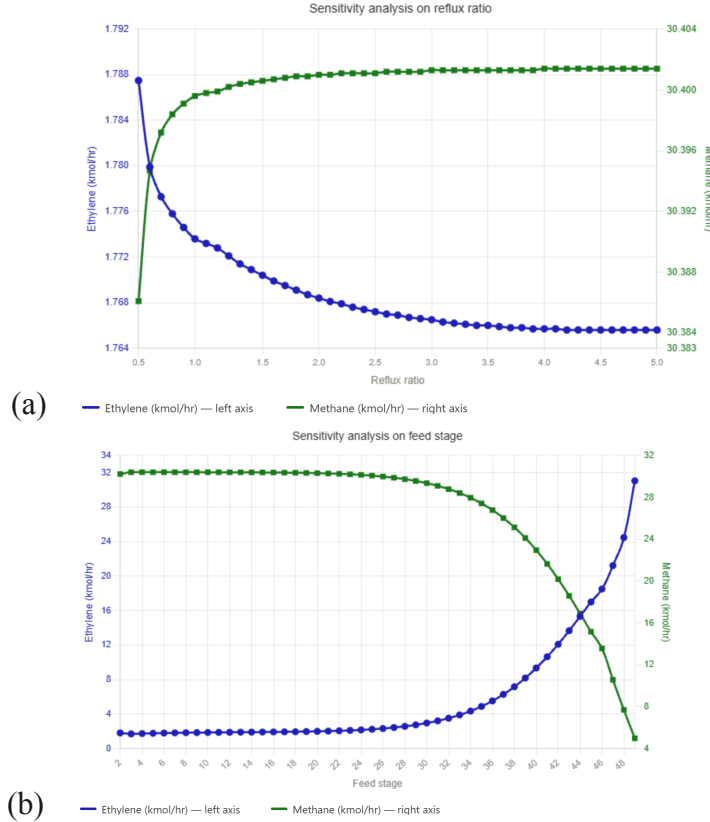


Figure 4. Sensitivity analysis on the (a) reflux ratio (b) feed stage.

Column Sizing and Hydraulic Design

The stripping vapour flow (3458 kmol/hr) is roughly 53 times greater than the rectifying vapour flow (65.8 kmol/hr). This extreme asymmetry is directly caused by the subcooled feed: the reboiler has to vaporize the 1925 kmol/hr of additional liquid added below the feed point, which significantly increases the stripping vapour load in comparison to what would be required for a saturated-liquid or vapour feed. Consequently, the stripping section regulates the reboiler duty as well as the column diameter.

The rectifying section, which is composed of a packed bed, is located between Stages 2 and 4. Trays would function well below their weep-point at these flow rates, so structured or random packing is far more suitable due to the rectifying section's low vapour and liquid traffic. The choice of BERL ceramic packing resulted in a packed height of 6.7 meters and a column diameter of 0.531 meters [37].

According to Sulzer design guidelines, the 20% safety margin applied to the hydraulic minimum height is justified by the known sensitivity of cryogenic packed columns to liquid maldistribution: at low temperatures, distributor performance is more difficult to guarantee and surface-tension effects are amplified. In the meantime, there are valve trays in the Stripping

Section between stages 5 and 49. For the high-flow stripping section, BALLAST-V4 valve trays were chosen, providing a column diameter of 2.565 m on 24 in tray spacing [38]. The design runs at 38% flooding, which is typical of the industrial demethanizer range of 35% to 45%.

Energy Analysis

The demethanizer's condenser and reboiler heat duties are shown in Table 17. Due to the comparatively small overhead vapor flow, which is almost entirely composed of methane, the condenser needs a duty of -0.228 MW, resulting in a modest refrigeration load at the top of the column. Due to the necessity of maintaining the necessary temperature gradient across the column and vaporizing a portion of the heavy C2+ bottoms product, the reboiler duty of 5.228 MW is much higher.

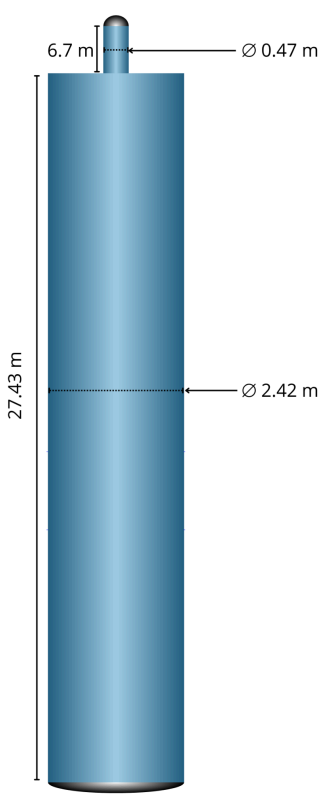
Table 21. Column Internals.

Parameter	CS-1 (Packed)	CS-2 (Trayed)	Units
Stage Initial	2	5	-
Stage End	4	49	-
Internal Type	Packed	Trayed	-
Packing/Tray Type	BERL Ceramic	BALLAST-V4	-
Packing Surface Area		-	m ² /m ³
Column Diameter	0.53	2.57	m
Number of Passes	-	3	-
Tray spacing	-	24	in
Packed Bed Size	6.7	-	m
Section Height	6.7	27.4	m
Min. Wall Thickness	45	11	mm
Wall Material [39]	SA-240 304L	SA-240 304L	-

Table 22. Heat Duty.

Condenser energy		Reboiler energy	
Heat duty, MW	-0.16	Heat duty, MW	4.71

Table 23. Design of T-104.

Demethanizer		
Diagram	Specification Details	
 Diagram of a vertical cylindrical distillation column. The total height is 27.43 m. The top section has a height of 6.7 m and a diameter of 0.47 m. The main body has a diameter of 2.42 m.	Flow Rates	
	Feed flow rate, kmol/hour	2074.33
	Distillate flow rate, kmol/hour	58.08
	Bottoms flow rate, kmol/hour	2016.25
	Column Configuration	
	Phase	Liquid-Vapor
	Calculation type	Equilibrium
	Condenser type	Partial-Vapor
	Reboiler type	Thermosiphon
	Reflux ratio	1.05
	Distillate to feed ratio	0.028
	Number of stages	50
	Feed stage	5

3.4 R-102 and R-103 Acetylene Hydrogenation Unit (AHU)

The selective acetylene hydrogenation unit (AHU) is the final step before the C₂ splitter (T-106) in the ethylene plant. The feed stream contains 572 ppm acetylene (C₂H₂), a steam cracking by-product consistent with the typical 0.04–0.10 mol% yield from ethane cracking [28]. Acetylene irreversibly poisons the Ti/Zr active sites of Ziegler–Natta and metallocene catalysts used in downstream polyethylene production, causing off-spec molecular weight distributions [28]. The AHU must therefore reduce acetylene to ≤5 ppm (polymer-grade specification), with a design outlet target of 27.5 ppm — a 5× margin that accommodates catalyst aging over a 360-day lead-bed cycle [28, 40].

Beyond purity, the AHU must meet three additional requirements: (i) ethylene selectivity ≥70% to minimise over-hydrogenation losses [41, 42]; (ii) pressure drop <0.5 bar to avoid penalising the compressor train [26]; and (iii) adiabatic bed temperature below ~80 °C to prevent catalyst sintering [41].

Reactor type selection

Four reactor archetypes were screened for selective C₂H₂ hydrogenation at the flow scale of the plant. Each option was evaluated against six criteria: capital cost, pressure drop, heat-management capability, selectivity at low partial pressure, maintainability, and commercial track record for tail-end service [26, 28, 42]. The outcome is summarised in Table 19.

Table 24. Reactor screening for selective C₂H₂ hydrogenation in tail-end service.

Reactor type	Advantages	Disadvantages	Suitability
Adiabatic packed-bed PFR (two-stage)	Simple design; low capex; mature industrial base (Lummus, KBR, BASF); no external heat input; predictable residence-time distribution; easy catalyst swap on lead-guard rotation.	Requires a second bed to reach ppm-level acetylene; small adiabatic ΔT needs control of inlet T and H ₂ injection to avoid runaway.	Selected. Industry-standard for tail-end Pd-Ag/Al ₂ O ₃ service.
Isothermal multitubular fixed bed	Tight temperature control; good selectivity under strong exotherm.	Adds a shell-side coolant circuit (cooling oil or boiling water); high capex; oversized for the modest heat release (~100 kW in lead bed).	Rejected — thermal duty too small to justify isothermal vessel.

Reactor type	Advantages	Disadvantages	Suitability
Slurry reactor (Pd on carbon, in solvent)	Excellent heat transfer; easy catalyst replacement.	Requires liquid solvent; complicates a gas-phase tail-end service; catalyst separation equipment needed.	Rejected — incompatible with vapour-phase feed at 25 bar, 60 °C.
Fluidised bed	Superb heat and mass transfer; continuous catalyst makeup possible.	Severe catalyst attrition; elaborate gas-solid separation; poor selectivity under low C ₂ H ₂ partial pressure; no commercial tail-end AHU on record.	Rejected — attrition-driven Pd losses would dominate operating cost.

The two-stage adiabatic packed-bed plug-flow reactor (PFR) with interstage H₂ injection is adopted because the heat release is small enough to be absorbed by the gas stream without active cooling, the Pd-Ag/Al₂O₃ pellet catalyst has a multi-decade commercial record in tail-end service [28, 41], and the lead-guard arrangement naturally handles Pd deactivation by rotating the lead and guard beds between maintenance cycles without interrupting production [40].

Reactor configuration: tail-end, two-stage with staged H₂

Selective hydrogenation can be implemented either upstream of the demethaniser (front-end, on the full cracked gas) or downstream of the depropaniser (tail-end, on the purified C₂ stream) [28, 42]. The tail-end configuration was selected for three reasons: (i) the hydrogen partial pressure is set independently by controlled injection, allowing precise control of the H₂:C₂H₂ ratio [42]; (ii) the catalyst sees a cleaner feed with no CO, H₂S or mercaptans, extending the deactivation cycle [41, 40]; and (iii) the outlet specification is easier to verify because the stream is essentially C₂H₄/C₂H₆/C₂H₂ [28].

Within the tail-end architecture, a **two-stage lead-guard configuration** with interstage hydrogen injection was selected over a single-bed reactor [42, 40]. In the two-stage layout, R-102 (lead) receives fresh feed and converts ~57 % of the acetylene, while R-103 (guard) finishes the hydrogenation to the 27.5 ppm specification. When the lead bed is judged to be near the end of its cycle (typically 360 days, see Section 3.11), the beds are rotated: R-103 becomes the new lead and R-102 is regenerated or replaced [40]. This rotation extends the mean time between full regens to ≈ 720 days and eliminates the risk of a polymer-grade excursion at the outlet [40]. Interstage H₂ injection is used to replenish hydrogen consumed in the lead bed and to keep both reactors near the optimal H₂:C₂H₂ ratio (2.89 in R-102 and 1.32 in R-103) [42].

Kinetics and design equations

The rate law adopted for design is the Langmuir–Hinshelwood–Hougen–Watson (LHHW) expression reported by Pachulski et al. [41] for Pd-Ag/Al₂O₃ at 333 K, which explicitly captures competitive adsorption of H₂, C₂H₂ and C₂H₄ on the Pd active sites:

$$r_1 = \frac{k_4 * K_1 * K_2 * P(C_2H_2) * P(H_2)}{(1 + \sqrt{K_1 * P(H_2)} + K_2 * P(C_2H_2) + \frac{P(C_2H_4)}{K_5}}) \quad (13)$$

The denominator term $P(C_2H_4)/K_5$ represents ethylene self-inhibition, which dominates the denominator at tail-end conditions because the stream is > 80 mol% ethylene [41, 43]. This inhibition is precisely what suppresses the ethylene over-hydrogenation pathway and delivers the high selectivity needed for polymer-grade output [41, 42]. Kinetic parameter values at 333 K are listed in Table 20

Table 25. LHHW kinetic parameters at 60 °C adopted from Pachulski et al. [41].

Parameter	Symbol	Value	Units
Acetylene rate constant	k ₄	5.26 E-3	mol/(kg·s)
Hydrogen adsorption constant	K ₁	13.00	bar ⁻¹
Acetylene adsorption constant	K ₂	107.00	bar ⁻¹
Ethylene inhibition constant	K ₅	7.40	bar
Catalyst bulk density	ρ _b	720.00	kg/m ³
Bed void fraction	ε	0.40	—
Mixture heat capacity (validation)	C _{p,mix}	55.00	J/(mol·K)

Energy balance.

Neglecting heat loss through the vessel wall, the bulk temperature rise from the exothermic acetylene and ethylene hydrogenations is:

$$\Delta T_{rise} = \sum (-\Delta H_{Ri}) \cdot n_{i,consumed} / (n_{mix} \cdot C_{p,mix}) \quad (14)$$

With $\Delta H(R1) = -176.6$ kJ/mol for main reaction and $\Delta H(R2) = -138.5$ kJ/mol for side reaction [44], the hand-calculated rise across R-102 is 3.24 °C, which agrees with Aspen Plus (3.14 °C) within 3 %

Ergun pressure drop

The bed pressure drop is computed with the Ergun equation [26, 45], which combines viscous (laminar) and kinetic (turbulent) terms for packed-bed flow:

$$\frac{\Delta P}{L} = \frac{150(\mu^* v^* (1-\varepsilon)^2)}{D_p^2 \varepsilon^3} + \frac{1.75(\rho^* v^{*2} (1-\varepsilon))}{D_p \varepsilon^3} \quad (15)$$

For a 3 mm catalyst pellet, $\varepsilon = 0.40$ [41], $\mu = 1.0 \times 10^{-5}$ Pa·s, $\rho = 29$ kg/m³ (C2-rich vapour at 25 bar, Aspen Plus), the Ergun coefficients evaluate to $A = 937.5$ Pa·s/m² and $B = 162\,238$ kg/m⁴, giving ΔP across both beds of 0.210 bar — well inside the 0.5 bar budget [26].

Reactor sizing

Sizing proceeds in three steps: (i) compute the catalyst mass required in each bed to meet the outlet acetylene target with the LHHW rate equation [41], (ii) sweep the vessel diameter over 1.2–4.0 m subject to an Ergun $\Delta P < 0.5$ bar [26] and the lead-bed aspect ratio $L/D \geq 0.50$ to avoid gas channelling [41], and (iii) pick the smallest diameter that satisfies both constraints. The sweep was coded in an Excel workbook.

The optimal diameter is $D = 1.90$ m. Adopting a common diameter for both beds simplifies fabrication, shared nozzle design, and spare-part stocking. The resulting geometry and duty are summarised in Table 21.

Table 26. Design summary for the two AHU reactors.

Parameter	R-102 (Lead bed)	R-103 (Guard bed)	Units
Reactor type	Adiabatic PFR	Adiabatic PFR	—
Operating pressure	25.00	25.00	bar
Inlet temperature	60.00	60.00	°C
Outlet temperature	63.10	60.90	°C
C ₂ H ₂ inlet	572.00	247.00	ppm
C ₂ H ₂ outlet	247.00	27.50	ppm
Acetylene conversion	56.90	88.90	%
Catalyst mass	2 100.00	5 000.00	kg
Vessel diameter	1.90	1.90	m
Bed length	1.03	2.45	m
L/D ratio	0.54	1.29	—

Parameter	R-102 (Lead bed)	R-103 (Guard bed)	Units
Heat release	98.90	40.00	kW
Ergun ΔP	0.06	0.15	bar
H ₂ :C ₂ H ₂ molar ratio (inlet)	2.89	1.32	—

The guard bed is $2.38 \times$ larger than the lead bed despite handling fewer absolute moles of acetylene. This is a direct consequence of the LHHW rate expression: at the guard-bed inlet the partial-pressure product $P(\text{C}_2\text{H}_2) \cdot P(\text{H}_2)$ is $11.7 \times$ smaller than at the lead-bed inlet, so the local rate is slower and more catalyst is needed to reach the polymer-grade specification. This catalyst-inventory skew, roughly 70 % in the final stage, is the well-documented signature of series-staged selective hydrogenation reactors [43].

Operating conditions

Temperature. The inlet was set at 60 °C after an economic optimisation over 40–80 °C. At 40 °C the Arrhenius-scaled rate is $3.1 \times$ slower ($E_a = 48.5$ kJ/mol [r1]), which would require $3.1 \times$ more catalyst and increase capital cost; at 80 °C the ethylene loss climbs to 0.21 % and coke formation accelerates, shortening the regeneration cycle to < 180 days [40]. 60 °C is also the industrial sweet-spot shown in figure 5. A high-temperature shutdown interlock at 85 °C gives a 22 °C margin above the maximum expected bed temperature [41].

Pressure. The reactor operates at 25 bar, the same pressure as the upstream C2 splitter feed stream, eliminating additional compression or letdown equipment [28]. An economic sweep over 15–35 bar confirmed that 25 bar minimises the combined cost of catalyst (lower at higher P), vessel wall (higher at higher P per ASME VIII Div. 1 circumferential-stress formula [46]), and upstream compressor (lower at lower P) [47]. At 25 bar and 60 °C the feed is fully vapour-phase, consistent with the adiabatic packed-bed assumption.

H₂ staging. The H₂:C₂H₂ inlet ratio is 2.89 in R-102 and 1.32 in R-103, set by the Aspen Plus sensitivity in Section 3.8 and consistent with the tail-end ratios recommended by Urmès et al. [42]. These two ratios together ensure: (i) no local hydrogen starvation in the lead bed, (ii) no excess hydrogen in the guard bed that would drive ethylene over-hydrogenation, and (iii) total hydrogen consumption aligned with the 2:1 stoichiometry plus losses [43]. The H₂ is a high-purity make-up stream injected via fail-closed FCVs with H6.3 interlocks .

Inter-stage cooling. The 3.1 °C adiabatic rise across the lead bed (60 → 63.1 °C) is removed by the inter-stage trim cooler E-106 before the guard bed. E-106 brings the stream back down to 60 °C so that R-103 starts at exactly the same inlet temperature as R-102. This reset is important because the guard-bed rate expression is evaluated at the same temperature point as the lead bed, which (i) simplifies kinetic validation by eliminating an Arrhenius correction between the two

stages, (ii) maintains the same 85 °C high-temperature interlock margin on both beds, and (iii) avoids a creeping upward drift of reactor temperature which would otherwise accumulate if the two beds were run in series with no interstage cooling.

Sensitivity analysis

Four sensitivity studies were run in Aspen Plus to confirm robustness of the design against operational drift: (i) split of H₂ injection between the lead and guard beds, (ii) total hydrogen make-up, (iii) feed temperature, and (iv) catalyst aging [42, 40]. Each study varied one parameter at a time while holding the others at their nominal values.

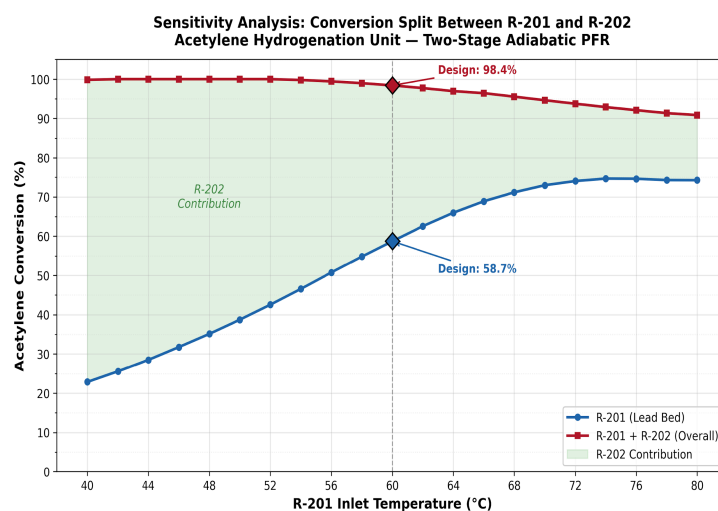


Figure 5. Conversion split between R-102 and R-103 as a function of lead-bed H₂ injection fraction.

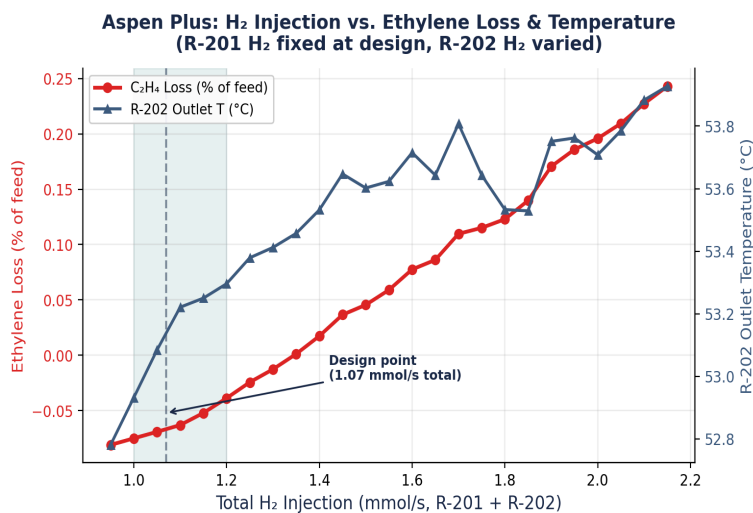


Figure 6. Aspen Plus sensitivity on total H₂ make-up.

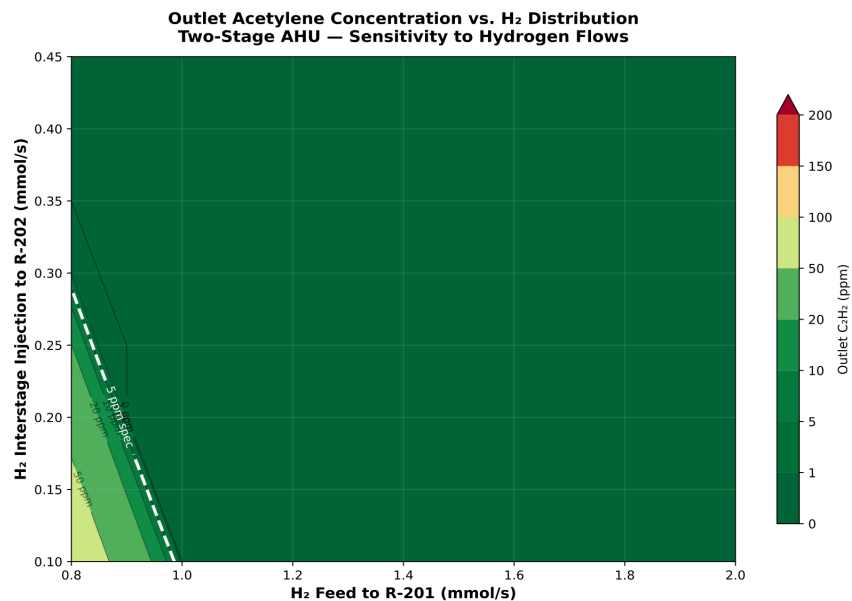


Figure 7. Outlet acetylene concentration (ppm) contour as a function of R-102 and R-103 H₂ injection rates.

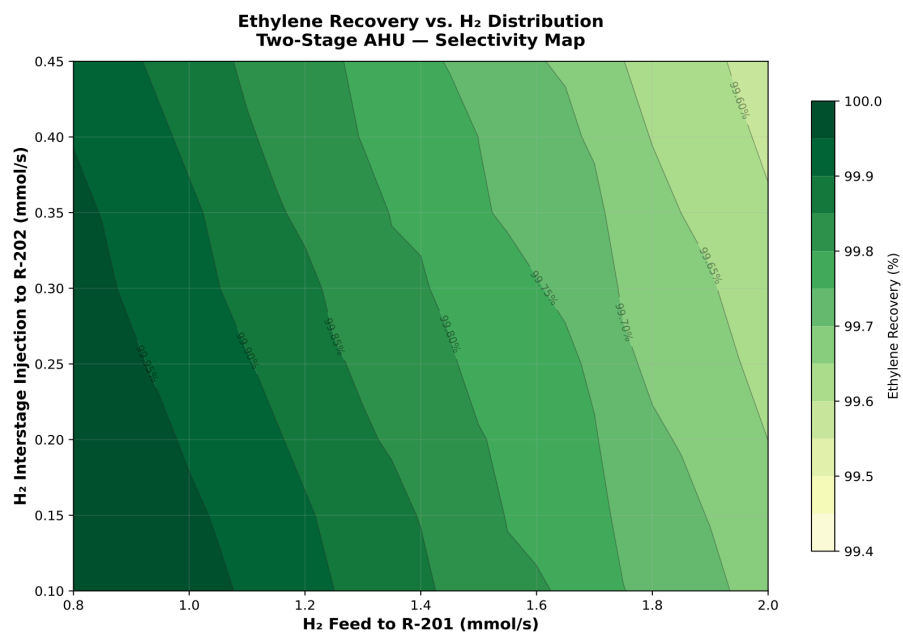


Figure 8. Selectivity (%) contour over the same H₂ injection grid.

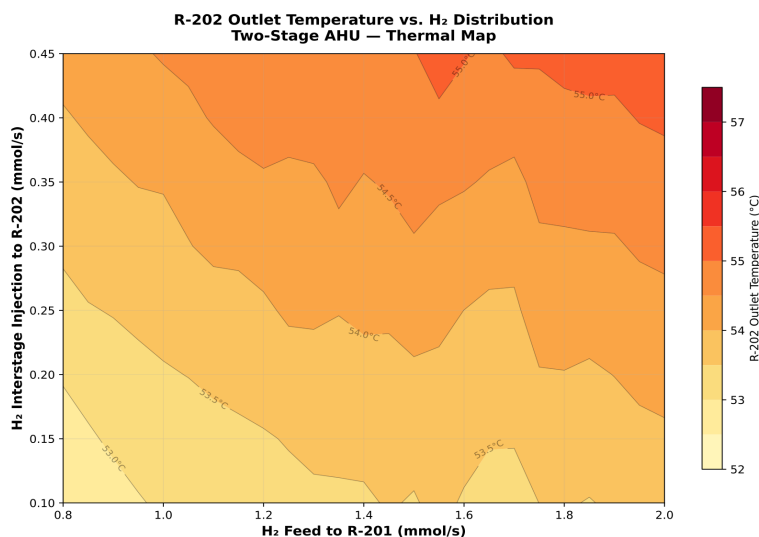


Figure 9. Outlet bed temperature contour.

The four figures together define a comfortably large operating window: the C₂H₂-outlet specification is met for lead-bed injection fractions between 0.58 and 0.78 and total make-up from 3.75 to 4.15 kmol/h, giving roughly $\pm 10\%$ headroom on every manipulated variable before the design has to be re-tuned.

Aspen Plus validation

The hand-calculated design was then validated against a rigorous Aspen Plus model using the RK-SOAVE equation of state and the built-in LHHW kinetics block [41]. The same feed composition, catalyst mass, and vessel geometry were supplied. Agreement on all key performance indicators is within 3 %, giving confidence in the design (Table 22).

Table 27. Hand calculation vs. Aspen Plus validation summary.

Parameter	Hand calc.	Aspen Plus	Agreement
R-102 adiabatic ΔT	+3.24, °C	+3.14, °C	3.20 %
E-106 inter-stage cooling	−3.10 °C (reset to 60.00, °C)	−3.14, °C	< 1.00 %
R-103 adiabatic ΔT	+0.87, °C	+0.92, °C	5.80 %
R-102 outlet C ₂ H ₂	247.00, ppm	246.90, ppm	< 1.00 %
Final outlet C ₂ H ₂ (R-103)	27.50, ppm	27.50, ppm	< 1.00 %
GHSV (R-102 / R-103)	659 / 280, h ^{−1}	659 / 281, h ^{−1}	< 1.00 %
Total catalyst mass	7 100, kg	7 115.00, kg	0.20 %
Ethylene loss	0.18 %	0.19 %	5.00 %

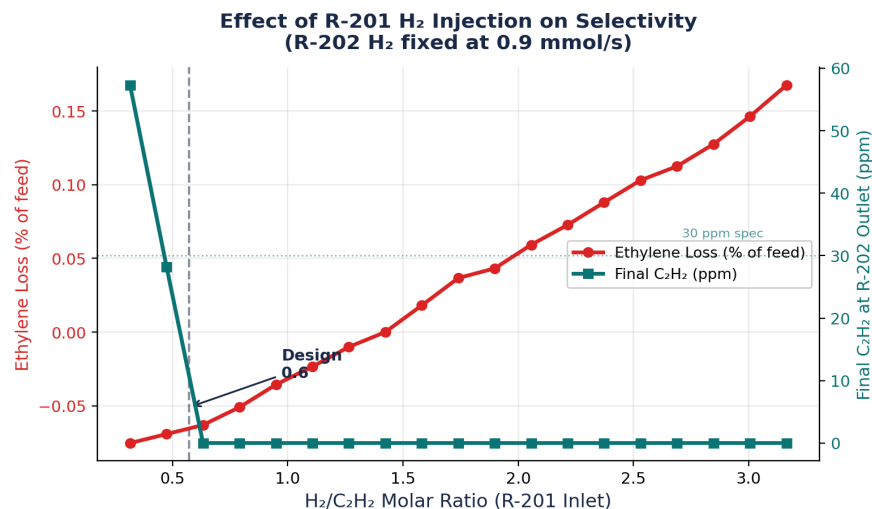


Figure 10. Aspen Plus result for R-102 (lead bed) at nominal operating conditions.

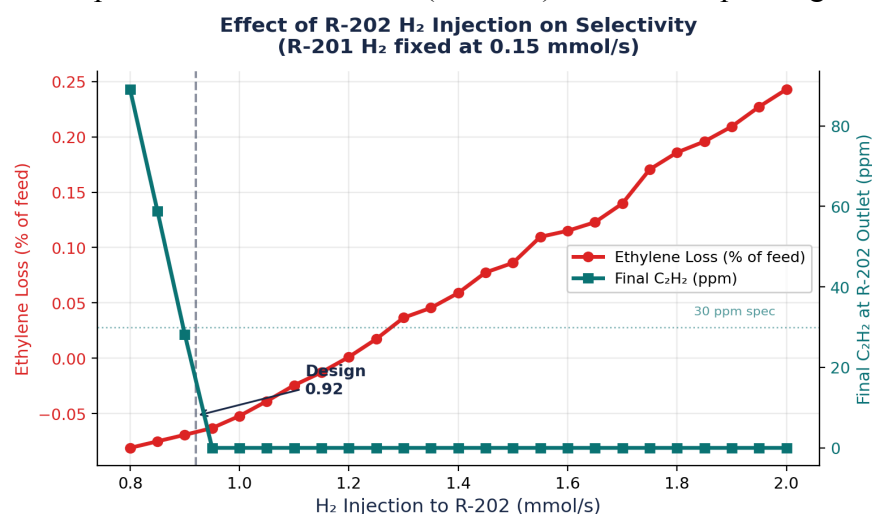


Figure 11. Aspen Plus result for R-103 (guard bed).

Vessel

Each reactor is a vertical cylindrical pressure vessel with 2:1 semi-elliptical heads per ASME Boiler & Pressure Vessel Code Section VIII Div. 1 [46]. The internal diameter is 1.90 m and the total tangent-to-tangent length is 4.5 m (R-102) and 5.9 m (R-103) — comprising the bed height plus 0.5 m of inert packing above the catalyst for gas distribution, 0.3 m below for support grid, and 1 m disengagement space for nozzle internals [26, 39].

Material

SA-240 Type 316L austenitic stainless steel is specified for all wetted surfaces [46]. 316L resists chloride stress-corrosion cracking from trace chloride contaminants in the feed, handles the mild

H₂/C₂ environment without embrittlement at 60 °C, and is compatible with Pd-Ag catalysts (no Fe leaching into the catalyst bed) [26, 45].

Wall thickness

The design pressure is set at 110 % of the 25 bar operating pressure, i.e. 27.5 barg, with a 10 % corrosion allowance [39, 46]. Using the circumferential-stress formula $t = PD/(2SE - 1.2P)$ with $S = 115$ MPa for 316L at 65 °C, $E = 0.85$ (radiographed longitudinal weld) [46], the required wall thickness is 18 mm. Rounded up to the nearest standard plate (20 mm), which also covers the expected 0.1 mm/yr corrosion rate over a 20-year design life [26].

Internals

A perforated distribution plate at the bed inlet ensures uniform gas flow; a stainless-steel support grid (40 × 40 mm square mesh) on ceramic balls supports the catalyst charge from below. A removable top manway (DN 600) permits catalyst loading and unloading. Thermocouples are distributed at three bed depths (inlet, mid-bed, outlet) for temperature profile monitoring.

Table 28. Mechanical specification sheet for R-102 and R-103.

Item	Spec
Design pressure / temperature	27.50, bar / 100, °C
Operating pressure / temperature	25.00 ,bar / 60, °C
Internal diameter	1.90 m
Tangent-to-tangent length (R-102 / R-103)	4.50, m / 5.90 ,m
Heads	2:1 semi-elliptical, both ends
Material	SA-240 Type 316L SS
Wall thickness	20.00, mm (incl. 2 mm CA)
Corrosion allowance	2.0, mm
Weld efficiency	E = 0.85 (spot-radiographed)
Catalyst	Pd-Ag/ γ -Al ₂ O ₃ , 3, mm extrudate
Catalyst charge (R-102 / R-103)	2 100, kg / 5 000, kg
Support internals	SS grid + 300, mm ceramic balls
Nozzles (inlet / outlet)	DN 150 flanged, ASME B16.5 class 300
Manway	DN 600 top, bolted
Insulation	75, mm mineral wool + SS cladding

Item	Spec
Design code	ASME VIII Div. 1 (2023 ed.)

Catalyst life cycle and regeneration

Pd-Ag/Al₂O₃ catalysts deactivate primarily through four mechanisms that dominate at different stages of the life cycle [41, 40]. Green-oil formation — oligomers of acetylene that condense on the Pd surface — is the first to appear and can often be reversed by steam–air oxidation [40]. Coke deposition accelerates above 80 °C and necessitates a full oxidative regeneration [41, 40]. Sulphur, arsenic and chloride poisoning from trace feed contaminants is largely irreversible and is controlled upstream with guard-bed arrangements [28]. Finally, Pd sintering — loss of active metal surface by sintering into larger Pd crystallites — dominates beyond the third or fourth regeneration cycle and is the ultimate end-of-life mechanism [41, 40].

According to Farsi et al. [41], the lead bed of a two-stage tail-end AHU is completely deactivated after a **360-day run length** while a significant fraction of the guard-bed activity is still retained. By rotating the lead and guard beds at 360 days — a standard operational practice [40] — the time between full in-situ regenerations is extended to approximately 720 days. Regeneration is performed in-situ with a controlled steam–air burn-off that removes the coke and restores the active metal dispersion, with a typical plant down-time of 48 hours [40].

3.5 C2 Splitter (T-106)

Function of the unit

The last step of the fractionation train would be separating the feed coming from the acetylene hydrogenation unit (Stream 43), ethylene (>99.9% purity), from mostly ethane as an overhead product in the C2 splitter. The process also requires low temperatures and a high reflux ratio, increasing the net work of the refrigeration step. Due to close volatility values between ethane and ethylene (ca. 1.1-1.2), the reflux ratio may be around 4 and stages ranging from 90 to 125 for polymer-grade polymer and 0.5% ethylene at the bottom stream [28]. The liquid ethylene can be stored in either semirefrigerated storage units working at 15 bar and -40°C or the fully refrigerated units at atmospheric pressure and -103 °C with varying volume [28]. The condenser and reboiler heat duties are integrated into propylene, ethylene or sometimes mixed gas vaporisation and condensation processes. Bottom stream consisting mainly of ethane and remaining hydrocarbons is sent to the mixer to be fed to the reactor R-101 as a recycle stream (Stream 49).

Working principle

Ethylene separation highly depends on the pressure, which can vary from 8 to 28 bars, ranging between low, medium and high pressure systems that alter operating temperature, pressure drop, viscosity and density of both vapor and pressure, which are critical factors in design calculations [28, 47]. Since there is a major trade-off between pressure and temperature, both consume a considerable amount of energy. Thus, the feed to the C2 splitter after acetylene hydrogenation is pre-cooled to -40°C, and the medium pressure system of 15 bars was chosen as the midpoint [48]. These conditions allow lower reboiler and condenser duties, smaller column diameter (ca. >5) and feasible relative volatility, which increases with pressure [47]. Higher relative volatility consequently leads to lower required $R_{\min}$ and the lower end of process tray number, decreasing the energy consumption.

For the pressure drop, it varies with the overall process pressure in the range of 0.25 to 1.2 [47, 49]. However, for design calculation purposes, the tray pressure drop was chosen at 0.16 psi or 0.011 bar, which leads to 0.7 bar as the overall pressure drop for 60-stage columns [50].

Design calculations

The following calculations were done for the process conditions of 15 bar and -40°C to separate 99.9% purity ethylene stream from an ethylene-ethane rich stream. The calculation process is similar to the previous separation columns with specific adjustments for the C2 splitter. The main steps include calculation of K-values for the species in feed with the Wilson equation, finding the minimum stage number ($N_{\min}$), minimum reflux ($R_{\min}$), reflux ratio (R), and actual stage number using the FUG method. Ethylene is the light key (LK), and ethane is the heavy key (HK).

The feed stream enters the splitter at 1957.20 kmol/hr, with an ethylene fraction of 0.64 and ethane at 0.36. There are other species in the stream, such as propane, acetylene and propylene, but their mole fraction is less than 0.0002. The -40°C or 233.15K is below the bubble point of the stream at 240K, meaning a liquid feed or q factor >1, which has to be noted to calculate the liquid and vapor flow for column dimension calculation [51].

K-value calculation

To find the relative volatility between LK and HK, the equilibrium constants (K) are calculated using the Wilson correlation (Equation 5) that utilizes critical and operating pressure and temperature to find K for each component in the feed, top and bottom streams. This equation is suitable for the systems under 34.5 bar containing light hydrocarbons [52]. The correlation coefficient was correlated to cryogenic conditions and was set as 3.762. The K-values were taken, and volatilities were calculated and averaged using the ratio of the K of the component to the K-value of HK. The mean volatility is the square of the product of the volatilities from the top and bottom streams [53]

$$\alpha = \frac{K_i}{K_{HK}} \quad (16)$$

Table 29. Relative volatility of the light key

Light key	Calculated relative volatility, α	Relative Volatility from Aspen, α
Ethylene	1.54	1.54

Shortcut FUG methods

The q factor of 1.0575 was calculated using the following equation based on McCabe-Thiele analysis, which correlated with the subcooled feed stream

$$q = 1 + \frac{C_{p,l}(T_b - T_f)}{\Delta H_v} \quad (17)$$

Where $C_{p,l}$ is the heat capacity of the liquid feed, T_b and T_f are bubble and feed temperatures, and ΔH_v is the latent heat of vaporisation [51].

The N_{min} was found with the Fenske equation (Eq. 6) and was equal to 24 stages. The Underwood root (θ) was found using the Goal Seek method using Equation 3 for R_{min} as a set formula equal to $1-q$ or -0.0575. The root has to lie between relative volatility values or between $1 < \theta < 1.5420$, which was 1.1398. The R_{min} is 2.8225, close compared to the Aspen R_{min} value of 2.85. From Equation 4, the R_{min} was multiplied by 1.3 to yield 3.73 as R. Leaving the R_{min} would lead to an infinite height tower, since it is close to the equilibrium curve. That is why, the value between 1.1-1.5 was chosen to balance the installation cost of the higher tray number and high energy intake for the reflux ratio.

To find the stage number (N), the Eduljee shortcut method was applied instead of Gilliland correlation, which essentially leads to the same X, Y values (0.1912, 0.4564) that lead to a stage number (N) of 46 (Eq.9-11). Although the true tray efficiency (E) should be taken directly from the manufacturer, a theoretical value can be calculated from the O'Connell correlation [50]. The method applies to the valve trays used in C2 splitters and uses the viscosity and relative volatility of the key component:

$$\eta = 0.492(\mu_f \times \alpha_{HK})^{-0.245} \quad (18)$$

This resulted in the E value equal to 0.81, which was used in Equation 8 to find the actual stage number (N_{actual}) equal to 56 stages.

The feed stage was found using the Kirkbride equation that uses the mole fractions of keys in feed, bottom and top streams:

$$\log\left(\frac{N_r}{N_s}\right) = 0.206 \log \left[\left(\frac{B}{D}\right) \left(\frac{x_{f,HK}}{x_{f,LK}}\right) \left(\frac{x_{b,LK}}{x_{d,HK}}\right)^2 \right] \quad (19)$$

From the equation, N_r is the number of stages above the feed with the condenser, and N_s is the number of stages with the reboiler [53]. The feed stage of 44 was calculated as follows and subtracted from the N_{actual} since Aspen counts from top to bottom.

$$N_s = \frac{N}{N_r/N_s + 1} \quad (20)$$

The sensitivity analysis was done to verify the stage number and feed stages to have the desired ethylene spec in the top stream (Figure 12). The analysis has shown that tray number of 66 and feed stage of 44 are the requirement for the lower reflux ratio value. The sensitivity analysis on the reflux ratio showed that 3.73 was the value for 0.999 recovery of ethylene in the top stream (Figure 12). The further increase of reflux ratio would give only a marginal increase for the ethylene molar fraction (Figure 13).

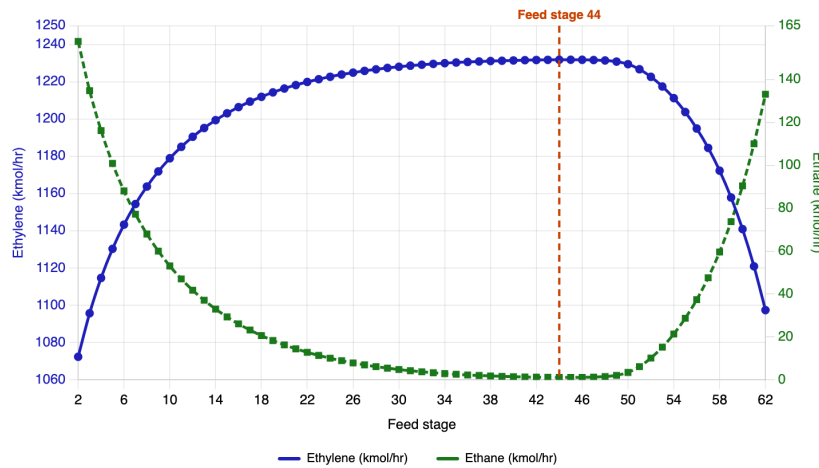


Figure 12. Sensitivity analysis on the stage design for ethylene recovery

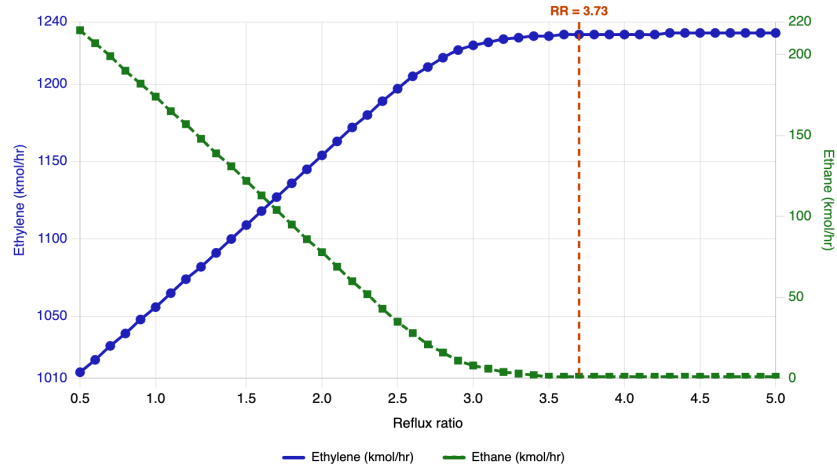


Figure 13. Sensitivity analysis on reflux ratio

Table 30. Calculation summary with main values

Parameter	Symbol	Value
Thermal condition of feed	q	1.06
Underwood root	θ	1.14
Minimum reflux ratio	$R_{\min}$	2.82
Actual reflux ratio	R	3.73
Stage number	N	46
Tray efficiency	E	0.80
Actual stage number	N_{actual}	63
Feed stage (from top)	N_s	44

C2 splitter sizing calculations

The column is divided into two sections: rectifying or top (Stages 2-44) and stripping or bottom (Stages 43-62). The column is trayed as they are more efficient for holding high liquid loads due to the subcooled feed stream and work better at higher operating pressure [54]. The total condenser is applied for its improved mass transfer efficiency at close volatility values and increased purity. With these assumptions, the sizing calculations are made with top and bottom section vapor and liquid flow calculations.

Table 31. Vapor and liquid flows in the top and bottom sections

Section	Flow rates	Formula	Value (kmol/hr)	Aspen (kmol/hr)
Top	Distillate (D)	DSTW	1233.04	-
	Liquid	R*D	4594.55	4594.89
	Vapor	L+D	5827.59	5827.59
Bottom	Bottom	DSTW	724.17	-
	Vapor	$(V_{top} + F(q-1)) * (\Delta H_{vap} \text{ ratio})$	5036.12	5483.51
	Liquid	$V_{bottom} + F$	5749.55	6193.24

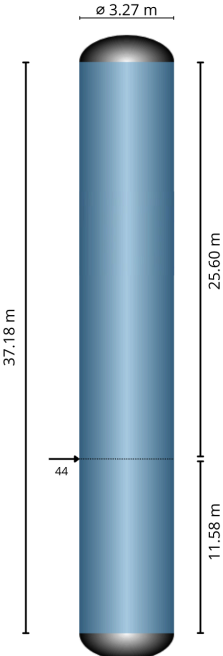
Since Aspen uses the enthalpy balance to measure the vapor and liquid flows in the sections, the correction factor was applied for the bottom section to bring the values closer. ΔH_{vap} ratio is the ratio of vapor and liquid enthalpy differences between the top and bottom. The enthalpy values are taken from the Profile section of the RadFrac.

$$Ratio = \frac{\Delta H_{vap, top}}{\Delta H_{vap, bottom}} = \frac{h_v^t - h_l^t}{h_v^b - h_l^b} \quad (21)$$

To determine the required net area, the actual vapor flow for both sections was calculated using the surface tension and vapor and liquid densities. The flow parameter was found with Fair correlation, and the C factor was found with the Souders and Brown curve equation [45]. Flood velocity is calculated considering the surface tension correction factor and is equal to 0.2926 m/s. From this value, diameters were found as 3.27m for the top and 3.10m for the bottom section, leading to almost one size diameter for the whole column. Therefore, to avoid the weak point at welding sites of different diameters, one common diameter of 3.27 was chosen.

Table 32. Column sizing and internals

Parameter	CS-1 (Trayed)	CS-2 (Trayed)	Units
Stage Initial	2	44	-
Stage End	43	62	-
Internal Type	Trayed	Trayed	-
Packing/Tray Type	BALLAST-V4	BALLAST-V4	-
Column Diameter	3.27	3.27	m
Number of Passes	4	2	-
Tray spacing	20	20	in
Section Height	25.60	11.58	m
Wall Material	SA516	SA516	-

Diagram	Specification Details	
	Phase	Liquid-Vapor
	Reboiler type	Thermosiphon
	Condenser type	Total
	Reflux ratio	3.73
	Number of stages	63
	Feed stage	44

The tray type is BALAST V-4, a valve tray used for C2 splitters, and the multi-pass trays are a conventional choice to avoid high weir cresting and uneven liquid flows [47]. Multiple passes distribute the liquid loads evenly across the tray, which is crucial for subcooled feed and medium to high-pressure columns. Tray spacing was chosen to be 24in or 609.6 mm to balance between the overall height of the tower and excessive downcomer [55]. The overall tower height is 37.2 m, below the 60m point and the wind load, while the ratio of height to diameter is ca. 12 (below 20), meeting the requirements to eliminate the wind load and foundation concerns [56]. SA516 carbon steel is a material of choice for its high yield and tensile strength that allows operation at 15 bar or higher [57].

Energy analysis

The heat duty of the C2 splitter consists of condenser duty (-16MW) and reboiler energy (16 MW). This balance of the whole duty can be explained by similar stage numbers in the rectifying and stripping sections and similar liquid and vapor flows.

Chapter 4. Minor Equipment Design

This chapter consolidates the design of all minor units in the plant that are not covered as individual major-equipment chapters. The scope covers the heat-transfer network (six heat exchangers E-101 through E-107), the three-stage compression train (C-101, C-102, C-103), the quench tower T-101, the molecular-sieve dryer T-102, the hydrogen separator T-103, the feed mixer M-101, the pressure-relief and control valves, and the four main storage tanks (raw-material ethane, product ethylene, propylene refrigerant, and quench-water surge). Each unit is designed to the heuristic / short-cut level required for Report 4 following Sinnott [26] and Perry [45], and the duties are validated against the Aspen Plus plant model.

Heat exchangers and heating / cooling units

The process has six heat-transfer services that are not covered in any major equipment chapter. They fall into two categories: fired/utility heaters (E-101, E-102) and recuperative heat exchangers (E-103, E-105, E-106, E-107). All duties were fixed by the Aspen Plus heat-and-material balance and the equipment selection was made per Sinnott heuristics [26] (shell-and-tube for $P > 7$ bar or $T > 200$ °C, welded-plate for cryogenic service), cross-checked against Perry's Chemical Engineers' Handbook [45].

E-101 Steam Boiler

E-101 is a packaged water-tube boiler that generates the dilution steam used upstream of the ethane-cracking furnace. Dilution steam plays two roles: it reduces the partial pressure of hydrocarbons in the coil to suppress coke formation, and it provides sensible heat that would otherwise come entirely from the furnace [58, 24]. The boiler is rated at the nominal duty shown in Table 4.1 with a firing margin of 20 % for transient start-up. The construction is carbon-steel water tubes with alloy-steel radiant headers per boiler design practice [26].

E-102 Feed Preheater

E-102 raises the combined ethane–steam feed from 93 °C to the 650 °C radiant-zone inlet [58, 23]. Because the stream temperature exceeds the safe limit for standard carbon steel, the tubes and bonnet are specified as high-alloy Incoloy 800HT (UNS N08811) to resist carburisation and high-temperature oxidation [22]. The exchanger is designed for a 0.3 bar pressure gain (rounded in Aspen) with fired-heater-type convection sections to recover heat from the cracking furnace flue gas [27].

E-103 First-stage Interstage Cooler

E-103 cools the cracked gas from the outlet of C-101 (201 °C) back down to 35 °C before C-102. Shell-and-tube, TEMA BEM type [26], with SS 316L tubes on the process side (high-pressure gas with trace H_2S / chlorides) and carbon-steel shell on the cooling-water side. A mild ΔP of 0.3 bar is tolerated per the intercooler pressure-budget heuristic [14].

E-105 AHU Feed Preheater

E-105 conditions the depropaniser overhead from $-14.87\text{ }^{\circ}\text{C}$ to $60\text{ }^{\circ}\text{C}$, providing a fully vapour-phase feed to the AHU (required for the adiabatic packed-bed assumption of Chapter 3 [41, 42]). A plate-frame configuration is specified to minimise hold-up and cope with the cryogenic-to-ambient temperature range [26]. Stainless-steel 304L plates and EPDM gaskets were selected for compatibility with the C2 hydrocarbon stream [29].

E-106 AHU Interstage Trim Cooler

E-106 drops the R-102 outlet from $63.16\text{ }^{\circ}\text{C}$ back down to $60\text{ }^{\circ}\text{C}$ before the guard bed R-103, resetting the lead-bed adiabatic rise. The duty is modest relative to the plant scale because the lead-bed adiabatic rise is limited to $\sim 3\text{ }^{\circ}\text{C}$ [41]. A simple shell-and-tube unit with cooling-water on the shell side handles the service [26].

E-107 C2 Splitter Pre-cooler

E-107 provides the cryogenic step that prepares the AHU outlet ($62\text{ }^{\circ}\text{C}$) for the C2 splitter ($-40\text{ }^{\circ}\text{C}$). Given the wide ΔT , a brazed-aluminium plate-fin exchanger (ALPEMA) is specified — the industry standard for ethylene-plant cold-boxes [28, 45]. The 15 bar pressure drop across the unit is absorbed by the C2 splitter feed path and does not need additional compression [47].

Table 33. Heat-exchanger and heating / cooling unit design summary.

Tag	Service	$T_{i\Box}\text{ (}^{\circ}\text{C)}$	$T_{ou\Box}\text{ (}^{\circ}\text{C)}$	Duty (kW)	ΔP (bar)	Material	Type
E-101	Steam boiler	107	200	824	10.50	CS / alloy steel	Water tube boiler
E-102	Ethane–steam preheater	93	650	39 905	-0.3	Incoloy 800HT	Fired convection
E-103	C-101 aftercooler	201	35	8 010	0.3	SS 316L / CS	Shell and tube
E-105	AHU feed preheater	-15	60	2 444	0.2	SS 304L	Plate-frame
E-106	AHU interstage trim cooler	63	60	100	0.1	SS 316L	Shell and tube
E-107	C2 splitter pre-cooler	62	-40	8 481	15	Brazed Al (ALPEMA)	Plate fin cold box

Pressure changers - three-stage compression train

The cracked-gas stream leaves the quench tower at 2 bar. The downstream separation section, dryer, depropaniser, AHU, and C2 splitter, needs the stream at roughly 32 bar [28]. Compression is therefore required, and because a single-stage unit with a compression ratio of 16 would exceed temperature and material limits, a three-stage intercooled train is specified [48]. Each stage is an electrically-driven centrifugal machine with a pressure ratio of around 2, consistent with industry practice for ethylene cracked-gas compressors [14]. An aftercooler (E-103 after stage 1, E-107 after stage 3 - both already described in §4.1) reduces the interstage gas temperature back to 35 °C before the next stage.

Table 34. Compressor-train design summary.

Parameter	C-101	C-102	C-103	Units
Inlet pressure	2.00	11.95	19.94	bar
Outlet pressure	11.95	20.00	31.94	bar
Inlet temperature	35.00	35.00	31.26	°C
Outlet temperature	201.09	81.45	73.65	°C
Vapour fraction	1.00	1.00	1.00	—
Polytropic efficiency	0.78	0.78	0.78	—
Shaft power	7 070.00	1 724.00	1 494.00	kW
Number of impellers	4.00	3.00	3.00	—

Materials: SS 316L for all wetted impellers and diaphragms; forged 4340 steel for the rotor shaft [26]. Each stage includes suction and discharge block valves (H3.1 HAZOP), a discharge PSV to flare sized per API 520 [59] (H3.3), and local vibration sensors (XSL / XSH) with an automatic trip at 2× baseline velocity [14]. A dry-gas face seal with nitrogen buffering replaces the older oil seal design [14], both reducing operating cost and eliminating hydrocarbon contamination of the seal-oil system.

Separators and dryers

T-101 Quench Tower

T-101 is a spray-type direct-contact quench tower positioned immediately downstream of the cracking furnace [60]. The 850 °C cracked gas is chilled to 35 °C in a single stage by a counter-current curtain of atomised water, condensing out the dilution steam and heavy pyrolysis tars while preventing further secondary reactions that would erode the ethylene yield [58, 24]. The spray configuration — without internal packing or trays — was chosen specifically to avoid fouling from coke and heavy aromatics that would rapidly plug a packed bed [60]. The cooling

water circulates in a closed loop, is polished of tars in an external API separator, and returned to the spray header [60]. The design parameters are in Table 4.3. Quench-water mass flow is sized via the sensible-heat balance

$$m_{qw} = Q / [c_p \cdot (T_{out} - T_{in})] \quad (22)$$

Table 35. Quench tower T-101 design parameters.

Parameter	Value
Operating pressure	2 bar
Inlet gas temperature	850 °C
Outlet gas temperature	35 °C
Heat duty	−69.14 MW
Quench-water inlet / outlet	25 °C / 82 °C
Quench-water circulation	1,044 t/h (290 kg/s)
Configuration	Spray-type, no packing / trays
Diameter / height	3.8 m / 16 m (sized per KLM heuristic 3 s residence time [60])
Material	Carbon steel with corrosion-resistant epoxy lining

T-102 Molecular-sieve Dryer

T-102 removes residual process water from the compressed cracked gas (outlet of C-103) before the cryogenic section [61]. Residual water in a stream that is subsequently chilled to −140 °C would freeze and plug the demethaniser internals; the specification therefore requires a dew point colder than −70 °C at 32 bar, equivalent to less than 1 ppm water by mole [61, 62]. A 3-Ångström zeolite (Zeolite 3A) molecular sieve is chosen because its 3 Å pore opening is selective for water over the C2+ hydrocarbons — it does not co-adsorb ethylene (kinetic diameter 4.2 Å), so the hydrocarbon stream is delivered bone-dry without any product loss [62]. The unit is designed as a two-bed swing adsorber (one bed drying, one regenerating) with a typical cycle length of 12 hours and regeneration at 250 °C with a slipstream of product gas [61].

Table 36. Dryer T-102 design parameters.

Parameter	Value
Operating pressure	31.92 bar
Inlet gas temperature	73.5 °C
Inlet water content	around 600 ppmv

Parameter	Value
Outlet water content	≤ 1 ppmv (-70 °C dew point)
Adsorbent	Zeolite 3A, 3 mm pellet
Bed configuration	Two-bed swing; 12-h cycle
Regeneration temperature	250 °C (product-gas slip)
Shell material	Carbon steel with 3 mm CA
Design standard	ASME VIII Div. 1

T-103 Hydrogen Separator (Cold Box)

T-103 strips the bulk of the hydrogen from the compressed cracked gas prior to the demethaniser [28]. Operating as a two-stage knock-out drum at about -100 °C, it exploits the large volatility difference between H_2 (boiling at -253 °C) and the $C2+$ components to recover a > 98 % pure H_2 overhead at 31.9 bar, while sending all the condensable hydrocarbons to the demethaniser bottom [28, 45]. Removing hydrogen at this point reduces the refrigeration duty of the cryogenic demethaniser by roughly 18 % and provides a ready H_2 stream for the AHU make-up [42]. The split of components is summarised in Table 4.5 (Aspen Plus balance).

Table 37. T-103 component split.

Component	Feed (kmol/h)	Top H_2 product	Bottom (to demethaniser)
Ethylene	1 281.350	0.000	1 281.350
Hydrogen	1 234.590	1 209.900	24.690
Ethane	710.340	0.000	710.340
Methane	30.280	0.000	30.280
Propylene	13.970	0.000	13.970
Propane	7.680	0.000	7.680
Acetylene	1.110	0.000	1.110
Water	0.002	0.002	0.000
Total	3 279.330	1 209.900	2 069.430

Mixers and control valves

M-101 Feed Mixer

M-101 is a simple in-line static mixer that blends the ethane feed from TK-102 with the dilution steam produced by E-101 before the combined stream enters E-102. The unit has no moving parts; it uses a 12-element helical-vane insert in a DN 400 pipe to achieve an outlet concentration uniformity of $\pm 1\%$ within 4 pipe diameters, consistent with standard static-mixer design guidance [26, 45]. The material is carbon steel lined with 3 mm of Inconel 625 to resist the 200 °C steam-wet environment [22].

Control and safety valves

The HAZOP study identified seven generic valve types required across the plant to manage flow, pressure, level, and emergency isolation. PSV sizing follows API Standard 520 [59], and emergency-isolation arrangements follow the recommended practice in Perry's Handbook [45]. Table 4.6 summarises their roles, fluid services, typical operating windows, and minimum counts.

Table 38. Valve catalogue

Valve type	Function / role	Fluid service	T (°C)	P (bar)	Fail mode	Min. #
Flow Control Valve (FCV)	Regulates flow of ethane, steam, quench water, refrigerant, H ₂	HC gas / steam / refrigerant / H ₂	-140 to +850	1 to 32	FC on fuel & H ₂ ; Fail-last on feeds	≥ 6
Pressure Safety Valve (PSV)	Protects vessels from overpressure — vents to flare	HC / H ₂ / steam	-140 to +850	2 to 32	Opens at set P; reseats on recovery	≥ 5
Non-Return Valve (NRV / CV)	Prevents reverse flow on ethane feed	Ethane / cracked gas	Ambient to 650	1 to 2	Passive — closes on reverse ΔP	≥ 1
Manual Isolation Valve (XV / BV)	Positive isolation for maintenance / ESD	Ethane / cracked gas	Ambient to 201	2 to 32	Manual	≥ 2
Level Control Valve (LCV)	Controls liquid level in quench-tower sump	Water / condensate	35 to 82	2	Fail-closed	≥ 1
Steam Control Valve (TCV)	Regulates reboiler steam	LP / MP steam	107 to 200	3 to 5	Fail-closed	≥ 1

Valve type	Function / role	Fluid service	T (°C)	P (bar)	Fail mode	Min. #
Refrigerant Control Valve (FCV)	Regulates refrigerant to demethaniser condenser	Propylene / ethylene refriger.	-140 to -40	5 to 20	Fail-closed (TALL interlock)	≥ 1

Storage tanks

Four primary storage systems were sized for the plant: (i) TK-101 ethylene product storage, (ii) TK-102 ethane feedstock storage, (iii) TK-103 propylene refrigerant storage, and (iv) TK-104 quench-water surge drum. The holding times are set by industry heuristics [26, 28]: 3 days of downstream buffer for product ethylene, 5 days of feedstock security for ethane, 7 days of refrigerant inventory, and a 30-minute surge buffer on the quench-water loop. The gross volume is obtained by dividing the net volume ($\text{mass} \times \text{holding time} \div \text{density}$) by the ullage factor 0.85 (API 625 / API 620 Annex Q cryogenic standards [63, 64]) and multiplying by a 10 % engineering margin [26]. The sizing basis and results are in Tables 4.7 and 4.8.

Table 39. Storage sizing assumptions and basis.

Assumption	Value	Basis
Plant operating hours	8 000.00 h/yr	Typical continuous olefins plant
Ethylene production rate	1 281.35 kmol/h	T-103 bottoms (Aspen)
Ethylene mass flow	35 941.00 kg/h	$\text{kmol/h} \times 28.05 \text{ kg/kmol}$
Ethane fresh feed	900.00 kmol/h	Industry typical for ethane cracker
Ethane mass flow	27 063.00 kg/h	$\text{kmol/h} \times 30.07 \text{ kg/kmol}$
Quench-water circulation	1 044 000.00 kg/h	Eq. 4.1
Ethylene density at -104 °C	567.00 kg/m ³	Perry's Handbook [45]
Ethane density at -89 °C	544.00 kg/m ³	Perry's Handbook [45]
Propylene density at -47 °C	609.00 kg/m ³	Perry's Handbook [45]
Ullage factor	0.85	API 625 / 620 Annex Q [63, 64]

Assumption	Value	Basis
Engineering margin	1.15	10 % on net volume [26]

Table 40 Storage tank sizing results. Boil-off gas (BOG) compression and N₂ blanketing are provided for TK-101 and TK-102.

Tank	Service	T (°C)	Flow (kg/h)	Hold time	Gross vol. (m ³)	Adopted (m ³)	Type / Standard
TK-101	Liquid ethylene	−104	35 941	3 days	6 170	2 × 3 250	Cryogenic flat-bottom, API 625 [63]
TK-102	Liquid ethane	−89	27 063	5 days	8 074	2 × 4 500	Refrigerated flat-bottom, API 620 Annex Q [64]
TK-103	Liquid propylene	−47	8 416	7 days	3 141	3 500	Refrigerated atm., API 620 [64]
TK-104	Process water	35	1 044 000	30 min	706	750	Vertical CS drum, atm. [26]

Chapter 5. Plant Location and Layout

5.1 Plant Location

The selection of the plant location depends on a number of factors: (1) options available in Kazakhstan, (2) service tariffs, (3) transportation, (4) political and strategic considerations, and (5) weather conditions. The choice of the location will impact the project's long-term economic viability and operational efficiency. These aspects to be discussed to choose an appropriate option.

Options available in Kazakhstan

In Kazakhstan Atyrau and Mangistau are centers of industrial development especially for the petroleum sector. Notably both regions have special economic zones which reduce taxes and simplify investment procedures. The following analysis will be concentrated on the comparison between two regions in order to identify the most suitable one.

Service tariffs

Determining the location considers service prices, namely water, electricity, heat supply and waste disposal tariffs. The comparison is made in Table 36 between Atyrau and Aktau cities (regional center of Mangistau). It is deduced that tariffs are comparable yet Aktau has less service expenses except waste disposal than Atyrau.

Table 41. Service tariff rates in Atyrau and Aktau cities

City	Water, USD/m ³	Electricity, USD/kWh	Heat supply, USD/GJ	Waste disposal, USD/m ³
Atyrau	0.42 [65]	0.073 [66]	0.82 [67]	3.63 [68]
Aktau	0.33 [69]	0.053 [70]	0.54 [71]	3.64 [72]

Transportation

Location of the plant should be near large deposits of natural gas in order to minimize costs on raw materials' transportation. In CIS region there are several areas which satisfy the following criteria. Most of them are placed in Azerbaijan, Turkmenistan, Uzbekistan and Kazakhstan, countries which also have the highest demand for ethylene in the region. Since Kazakhstan is in the middle of the region, the oil and gas industry is already developed and it is politically stable, this country is the most preferable among them. When comparing Atyrau and Aktau, Atyrau is

best for inbound logistics, due to its proximity to the major gas fields, while Aktau is optimized for outbound transportation, due to port infrastructure in Caspian Sea. Overall, since a major ethane production plant is centered in Atyrau to reduce the transportation fee, Atyrau is preferred [73].

Political and strategic considerations

Table 37 summarizes taxations and tax benefits for industries operating in Special Economic Zones (SEZ) "National Industrial Petrochemical Technopark" in Atyrau, Aktau, and Kazakhstan's standard taxation system. Overall, locating the facility within SEZ has a lot of advantages in terms of taxation.

Weather conditions

In terms of weather conditions both Atyrau and Aktau have hot summers, and mild winters in comparison with other regions of Kazakhstan, it will allow the facility to work in winter. Average temperatures in winter time in Atyrau do not go lower than -10°C, and in Aktau do not go lower than -5°C, which prevents the units and piping from freezing. This will minimize the operational costs for these units and increase the number of production days. Weather conditions of Atyrau and Aktau are presented in Figure 14.

Table 42. Tax obligations in SEZs and Kazakhstan standard taxation system.

Name	SEZ "National Industrial Petrochemical Technopark" [74]	SEZ "Seaport Aktau" [75]	Standard taxation in Kazakhstan
Corporate income tax	0%	0%	20% [76]
Land tax	0%	0%	The tax amount differs based on location
Property tax	0%	0%	1.5% [77]
Value added tax (VAT)	0%	0%	16%[76]

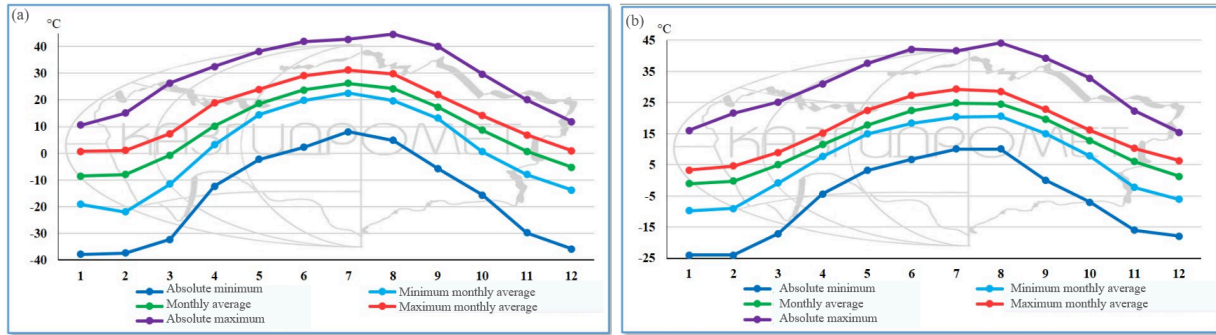


Figure 14. Weather conditions in Atyrau (a) and Aktau (b) [78, 79]

Choice of location of the plant

By considering the factors such as (1) options available in Kazakhstan, (2) service tariffs, (3) transportation, (4) political and strategic considerations, and (5) weather conditions SEZ "National Industrial Petrochemical Technopark" was chosen as a location for the plant.



Figure 15. Surroundings of the SEZ "National Industrial Petrochemical Technopark".

SEZ "National Industrial Petrochemical Technopark" was chosen as the location for the plant. As illustrated in Figure 15, the facility gains several advantages from this location:

- A well-developed transport network, including roads all over the territory and railways, ensuring efficient logistics. The plant is 32 km from Atyrau city by Atyrau-Dossor highway and the closest and biggest railway station is Atyrau Railway Station. The Karabatai Railway Station can be used for supplying the future industrial zone.
- Proximity to a river, enabling reliable water supply and additional transport options.

To achieve the targeted 300,000 tons per year, 60 hectares should be sufficient, it provides fire gaps and blast zones for safety, future perspectives for expanding capacity, and operational

efficiency by accommodating warehouses and administrative buildings. The location is shown in Figure 16. Together with allowing for the full implementation of a full-scale production facility, additional land is available for further expansion, this site provides the scale and flexibility required for this project.

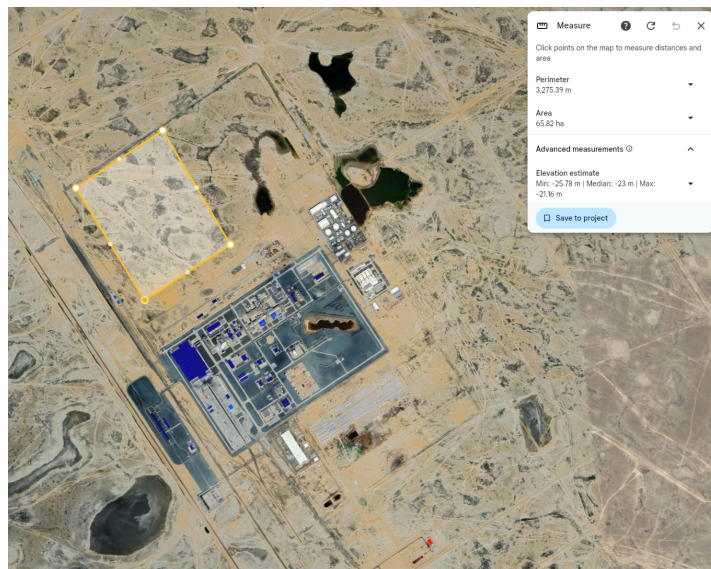


Figure 16. Ethylene plant location.

5.2 Plant layout

Layout zones

Plant layout was developed based on the general principles and process safety requirements. The layout is divided into several zones according to their purpose and risk level shown in Figure 17.

- Red zone - core production area and storage tanks, which are associated with the highest safety risks due to high-temperature processes and toxic chemicals.
- Orange zones - utilities, laboratories, fire station, control rooms, and machinery operations. With lower safety risks.
- Green zones - administrative buildings, canteen, parking, and other facilities (e.g. first aid stations, changing rooms, hospital, washrooms, and restrooms). These zones are separated from production facilities, to minimize personal exposure and create low-risk areas.
- Dashed white zones - future expansion zones
- Blue zones - emergency water.

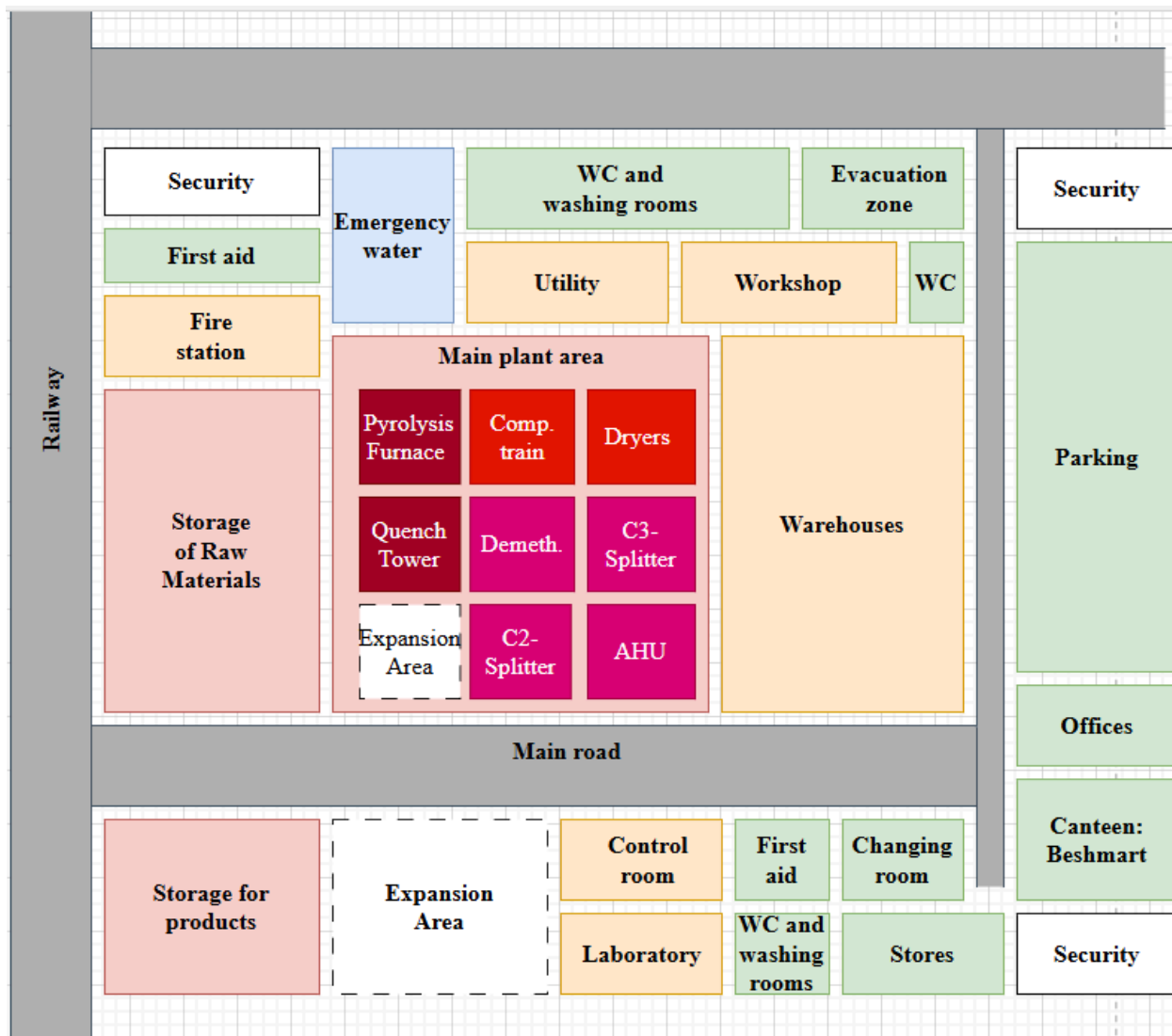


Figure 17. Plant Layout.

Production and Storage Tanks zones

To improve overall safety and avoid cross contamination of the chemicals. The storage tanks were placed closer to the main road within the designated area, allowing faster loading and unloading of raw materials and products, minimizing the transportation time and overall logistics. The layout specifies the number of storage tanks per species. There are for natural gas, water, and quench water in storage of raw materials and for ethylene and propylene tanks for products.

Low-risk zones

To facilitate comfort and safety of human personnel, the canteen, parking areas, and offices are located farther from the production areas, whereas washrooms and changing rooms are located near work areas, supporting hygiene and comfort.

Emergency and Safety zones

Emergency zones: first aid, emergency water, evacuation, and fire station are located nearby. The plant has three security checkpoints at the borders of the facility area to reduce the risk of unauthorized entrance and improve access control.

Future expansion

The layout includes spare space for future storage and plant area, allowing future expansion. This provides necessary room for scaling up operations or adding new units without disrupting workflow.

Chapter 6. Process Safety and Environment Management

6.1 Process Safety

Chemical plants concentrate many hazards inside, which leads to undesirable outcomes like staff harm, environmental distraction or economical losses. It can be noted that there are many sources of a Major Accident Hazard (MAH) on site including chemicals, electricity, physical impact, equipment malfunction, and process design error. Studying possible hazards in the ethylene production reduces risk of undesirable consequences, and minimizing them is the first priority of plant design.

Explosions and fire risks

Ethylene, ethane, methane and hydrogen are extremely flammable gases. Autoignition occurs at 543 °C, 510 °C, 540 °C, and 580 °C, respectively (Table 19) [80]. They all form an explosive mixture with air. The risk of explosion on the plant always remains on the highest level because the possibility of Loss of Contamination should be considered anytime. In the case of a major accident flash fire or vapour cloud explosion should be expected. Additionally, without adequate cooling while an affected external heat Boiling Liquid Expanding Vapor Explosion (BLEVE) occurs.

Toxicity

Ethylene, and the rest gases are considered as relatively non-toxic, however, at high concentration in air causes asphyxiation. It is a condition when the body does not receive sufficient amounts of oxygen. Symptoms include paralysis of the respiratory center which after long exposure leads to lethal cases [81]. Workplace exposure limits are set that at any given moment the concentration of oxygen cannot be less than 19% [82].

HAZOP analysis

For Safety analysis Hazard and Operability Study (HAZOP) applied. A HAZOP is a structured and systematic risk assessment technique used in the chemical and process industries to identify potential hazards and operability problems within a facility. HAZOP enables evaluating causes, consequences, and existing safeguards, and to recommend corrective actions before hazardous scenarios materialise. The demethanizer column T-104 is presented here as a representative example of the HAZOP findings for this ethylene production facility.

High pressure in the column in T-104 is one of the deviations determined by the HAZOP study. The reason for such a condition in the process is the inability of vapour to condense, causing uncondensed methane and hydrogen, which cannot escape through the column overhead. The initial risk was rated 10 (likelihood 2, severity 5), placing this deviation in the high-risk category requiring immediate action. If this deviation takes place, there will be severe consequences since column shell overpressure will lead to its destruction and cause a massive discharge of cryogenic methane and hydrogen, with possible flash fire or explosion.

The measures currently in place include Pressure Alarm High (PAH), Pressure Safety Valve (PSV), and the high-pressure Emergency Shutdown System (ESD). While these provide a baseline level of protection, the residual severity of 4 indicates that the consequences remain significant even with these measures in place. Two recommendations include installing an independent Pressure Alarm High-High (PAHH) interlock on T-103 overhead and introducing a Pressure Alarm Low (PAL) and Flow Alarm Low (FAL) for the refrigerant to detect any defects in it, thus, preventing vapours from condensing. Following implementation of these measures, the residual risk is reduced to 4 (likelihood 1, severity 4), representing an acceptable risk level within the facility's risk matrix.

Regulations and legal considerations

In order to produce the ethylene the plant should comply with local laws and regulations. In the Republic of Kazakhstan GOST documents serve as the main government source for regulations. The production should satisfy GOSTs in product specification, testing, piping, pressure equipment, area classification, hazard communication and occupation safety. Below is a list of the most important documents with which the plant should comply.

Table 43. Summary of Applicable GOST Standards for the Ethylene Production Plant.

Category	Standard	Scope
Product & Testing	GOST 25070-2013	Ethylene. Technical specifications
Product & Testing	GOST 24975.1-2015	Ethylene & propylene.

Piping & Valves	GOST 32569-2013	Steel process pipelines. General requirements
Hazardous Areas / Ex Equipment	GOST 31610.10-1-2022	Classification of zones. Explosive gas atmospheres
Occupational Safety (SSBT)	GOST 12.1.004-91	Fire safety. General requirements
Waste Treatment	GOST 30772-2001	Resource conservation. Waste management.

6.2 Environmental Management

Fauna & Wildlife

Baseline studies have established the absence of Red Book, rare, or endemic species on the proposed site. The main risks to local fauna include dust generation during construction and maintenance, and low-frequency noise from process equipment affecting birds and mammals nesting or burrowing nearby.

Mitigation measures include: motion-triggered camera trap monitoring to detect protected species entering the perimeter; a "no destruction of burrows" policy during excavations to protect steppe mammal populations; and a facility light pollution study to minimize light spill into the surrounding environment.

Soil & Land Resources

Soil compaction from traffic and foundation works is managed through designated traffic routes and hardstandings. Salinization risk from process water and chemical storage is controlled through impermeable liners, drainage collection systems, and bundled secondary containment. The primary threat to soil integrity is hydrocarbon spillage from storage tanks and pipework, mitigated by underground leak detection systems around hydrocarbon storage areas and a routine soil monitoring program for pH and Total Petroleum Hydrocarbons (TPH).

Water Resources

There is no direct discharge route to the Zhaiyk River or its tributaries. Two residual risks remain: hydrocarbon migration into the shallow aquifer through soil transfer, and insufficient water recycling efficiency leading to elevated consumption and discharge volumes.

The major wastewater streams produced by the plant include the quench water used in the effluent cooling from the cracking furnace, condensate from the process obtained after steam separation, and blowdown from cooling towers. The quench water contains high concentrations of hydrocarbons and suspended solids and needs pretreatment before being sent to the main effluent stream. Process condensate, on the other hand, is clean enough to be reused as boiler feed water once it undergoes stripping of hydrocarbons and ammonia.

The treatment of the effluents takes place in four steps, including physical separation using an API oil-water separator to separate free hydrocarbons and suspended solids, chemical precipitation to remove heavy metals and emulsified substances, biological oxidation to break down organic material, and finally filtration. Wastewater quality monitoring includes continuous monitoring of pH, COD, and TPH, and periodic BOD₅ monitoring.

Emission control

Ethylene production via steam cracking of ethane releases substantial quantities of carbon dioxide, nitrogen oxides, and volatile organic compounds, the management of which is critical for regulatory compliance and reducing the facility's environmental burden [83].

Aspen Plus simulation results indicate a total CO₂-equivalent emission rate of 23,417.6 kg/hr, corresponding to an annual load of 205,178 t/yr and a GHG intensity of 677 kg CO₂e per t of ethylene produced. The associated carbon cost amounts to \$585.44/hr, or approximately \$5.13M per year. The primary source is hydrocarbon combustion in the R-101 and associated waste streams. To mitigate these emissions, the plant can adopt carbon capture and storage to sequester CO₂ underground [84], or carbon capture utilization to convert it into value-added products such as methanol [85]. Transitioning to low-carbon fuels and integrating renewable energy into grid operations can further reduce the facility's overall carbon footprint [85].

Meanwhile, Nitrogen oxides are generated as a byproduct of combustion. Low-nitrogen oxide burners suppress their formation by regulating flame temperature and the air-fuel mixing ratio. For post-combustion treatment, selective catalytic reduction or selective non-catalytic reduction converts nitrogen oxides into nitrogen and water vapor [86], ensuring compliance with the Kazakhstan Environmental Code [86], ISO 14001 [87], and European Reference Documents (BREF) [83].

Table 44. Summary of emission and their sources

Block ID	Block Type	Duty	Usage	Cost	CO₂ Emission Rate
E102	HEATER	55.66 MW	125.23 t/hr	\$11,135,668/yr	11.85 t/hr
E101	HEATER	15.82 MW	229,035 t/yr	\$4,803,232/yr	35.78 t/yr
B6	HEATER	2.41 MW	34,414 t/yr	\$743,131/yr	114,490 t/yr
COMPRES1	COMPR	6.99 MW	6.99 MW	\$4,747,872/yr	19,123t/yr
COMPRES2	COMPR	1.70 MW	1.70 MW	\$1,157,595/yr	4,662 t/yr
COMPRES3	COMPR	1.49 MW	1.49 MW	\$1,015,221/yr	4,089t/yr
B7	PUMP	0.01 MW	0.01 MW	\$7,308/yr	29.44 t/yr

Chapter 7. Total Investment and Profitability

This section is mainly focused on the capital and operating cost estimation, profitability and risk analysis of the plant at the production rate of 300 kt/year of ethylene in Kazakhstan special economic zone (SEZ). The main assumptions are that the plant runs 7621 h/year or 87% on stream factor. The construction starts in the year of 2028 and takes two years, while operation starts in 2030 with a nine year projection of cash flow [88, 89]. The units for capital are in USD in the 2025 rate with an inflation rate of 11.7%/year for revenues and operating costs as stated in the Ministry of National Economy in their chemical industry outlook [89]. The location of the plant ensures 0% corporate income tax for 25 years as a Category C based on the capital investment value [90].

7.1 Price of feedstock and Final products

The case of ethane cracking is based on the ethane gas feed cost and the selling price of the polymer-grade ethylene to downstream converters. Byproducts such as the H_2/CH_3 fuel gas and mixed C_3+ streams are also considered in the revenue stream. In Kazakhstan exact ethane feedstock price is not specified, as it is usually project dependent or negotiated value due to construction of polyethylene complex with feed supply from KazMunayGas Gas separation complex [91]. Although, \$80/t was stated as the value of the ethane gas in Kazakhstan, which is applied in cost calculations [93]. The ethylene selling price is set at \$844/t, which is consistent with the market price in North-East and South-East Asia ranging between \$822-880/t in 2024 [94, 95, 96]. The byproducts are set as \$50/t as a fuel gas, lower value than the market price but most of the gas is directed to be burnt on-site of the plant. Propane/propylene mix price is also set below the market price due to mixing of the outlet stream from depropaniser.

7.2 Cost of equipment and storage tanks

Equipment purchase costs were estimated via the cost-curve method of Sinnott and Towler [94], in which the free-on-board equipment cost is given by the following formula:

$$C_e = a + b \cdot S^n \quad (24)$$

There the C_e is the equipment cost, a and b are correlation constants such as material, installment factor, S the sizing parameter specific to the type of equipment and n is the scaling exponent or 0.6 in this case. Most of the equipment costs were provided by the Aspen analysis, while several C_e had to be estimated using the aforementioned Equation X. The installed cost was written using the formula below:

$$C_{installed} = C_e \cdot \frac{CEPCI_{cur}}{CEPCI_{base}} \cdot LF \cdot IF \cdot MF \quad (25)$$

The values for the CEPCI were taken as 820 for the current year as 2022 annual value was 816, while the base CEPCI set at 600, consistent with 2019-2020 averages [95]. Therefore, the escalation factor is 1.3667. The location factor is set as 1.4 for the Central Asian remote region, where the US is a reference point at 1.00 and the Western Europe is at 1.20 [94]. The installation

and material factors are taken from the hand-factor ranges for the specific equipment type and the material utilised according to the composition inside the equipment as well as operating conditions. Condensed equipment list, their equipment and installed costs are shown in the Table K1. The overall purchasing value was calculated to be \$51.2M, while the total installation cost was set at \$330.3M. A detailed table for each equipment is provided in the Appendix.

Table 45. Condensed equipment with equipment and installation costs

Equipment	Equipment Cost (USD)	Installation Cost
Compressors	\$13,717,400	\$69,128,877
HEX/coolers	\$6,439,928	\$56,203,075
Pump	\$72,100	\$551,805
Reactors	\$8,946,500	\$57,608,362
Storage tank	\$11,035,833	\$73,236,022
Columns	\$11,020,000	\$73,556,073
Total	\$51,231,761	\$330,284,214

This table presents the storage tank sizing and cost calculations based on flowrate, storage time, density, and required tank volume for each stream. The largest tank costs are associated with ethane feed and ethylene product storage, mainly because of their high required volumes of 8602.9m³ for ethane gas feed and 2,923.4m³ with liquid ethylene product and the use of more expensive low-temperature materials such as 9% nickel steel. In contrast, smaller auxiliary tanks such as oily water, drain water, and C₃ gases have a much lower cost contribution. The calculations are shown in Table K2.

Table 46. Storage tank cost estimation

	S-101	S-102	S-103	S-104	S-105	S-106
Description	Ethane	Oily Water	Drain Water	Methane	C3 gases	Ethylene
Flowrate	39000	19024	1442	592	918	34593
Time, days	5.0	0.5	0.5	1.0	1.0	2.0
Mass, kg	4,680,000	228,288	17,303	14,208	22,032	1,660,464
Density, kg/m ³	544	984	956	24.9	600.0	568
Volume, m ³	8,603	232	18	628	37	2,923
Tank Type	API 620 R	API 620 R	API 650	API 620 R	ASME Section VIII	API 620 R
Material	9% Nickel Steel	A36 Carbon Steel	A36 Carbon Steel	9% Nickel Steel	SA-516	9% Nickel Steel
Reference Cost	\$4,000,000	\$115,000	\$115,000	\$760,000	\$85,000	\$3,000,000
Total Cost	\$5,466,667	\$157,167	\$157,167	\$1,038,667	\$116,167	\$4,100,000

7.3 Capital Investment Estimation

The total fixed capital investment (FCI) is obtained by adding the outside-battery-limits (OSBL) support facilities, engineering services, contingency and working capital on top of the inside-battery-limits (ISBL) installed cost of \$330.28M established in Section 7.2. The percentages applied to the ISBL value follow the ratio approach of Sinnott and Towler for grass-roots petrochemical complexes, with a reduced contingency that reflects the high confidence in the Aspen-based equipment cost after CEPCI, location and hand-factor corrections have already been embedded in the installed-cost line.

Support facilities (OSBL) are set at 20% of ISBL, giving \$66.06M. This line covers the utility generation units including cooling-water circulation, the three-stage refrigeration loop, steam and imported-power substations, together with flare and relief systems, site buildings, roads, the central control room, tankage interconnections and off-site infrastructure that lie outside the main process battery limits but are required to keep the cracker operational.

Engineering services are set at 15% of ISBL, or \$49.54M. This covers the EPC contractor fees for detailed process and mechanical design, procurement management, construction supervision and commissioning support. A premium over the US-Gulf-Coast baseline is retained in the percentage because the Atyrau SEZ site is remote and therefore carries higher mobilisation costs and a larger share of expatriate man-hours, consistent with the 1.4 location factor already applied in Section 7.2.

A contingency reserve of 2% of ISBL, equal to \$6.61M, is retained to absorb minor scope growth and cost-escalation risks during construction. This value is intentionally lower than the 10–15% Class-4 AACE contingency typically applied at feasibility stage, because the underlying equipment cost already carries the 1.3667 CEPCI escalation factor and the 1.4 location factor, which together remove most of the macro-scale cost uncertainty. The residual risk being covered is limited to construction-productivity variation and minor scope additions.

Working capital of 15% of ISBL, or \$49.54M, is injected in the first construction year to fund the initial inventory of ethane feed and saleable ethylene, spares, accounts receivable and the operating cash float required before the first full year of revenue is collected. Consistent with standard practice, working capital is treated as non-depreciable and is assumed to be recovered in full at the end of the ten-year economic horizon.

Summing ISBL, OSBL, engineering services, contingency and working capital gives a total fixed capital investment of \$502.03M. The CAPEX is phased across the two construction years on a 33.3% / 66.7% split, equal to \$167.18M in 2028 and \$334.86M in 2029, which follows the

progress-payment profile typically negotiated with EPC contractors for ethylene plants of this scale.

7.4 Fixed cost

Fixed operating costs comprise direct labour, supervision, salary overheads, maintenance, property tax and insurance, environmental charges and general administrative overhead. Labour headcount is computed from the Alkayat–Gerrard correlation [96]:

$$N_{ol} = (6.29 + 31.7 \cdot P^2 + 0.23 \cdot N_{np})^{0.5} \quad (25)$$

Where P is the number of particulate-handling steps and N_{np} is the number of non-particulate process units. For 0 as a value of P for the gas-phase cracker and N_{np} 10 for the ethylene plant, the N_{OL} was equal to 2.93 operators/shift. Although the Turton coverage multiplier gave 13 operators/year as a lower bound, the value of 28 was set for the operating labor, which is consistent with the plants with 300kt/year production rate [97]. The wage was set at \$14500/year as an average wage for the Atyrau-region [98]. With the supervision (25% of direct labour cost), salary overhead (40% of labour and supervision), maintenance (3% of ISBL), insurance (0.5% of ISBL), general administrative expenses (65% of labour and supervision), the overall fixed operating cost is set to \$12.7M per year (Table 42).

Table 47. Total fixed operating expenses breakdown

Item	Amount, US \$/yr
Direct operating labour	406 000
Supervision	101 500
Salary overhead	203 000
Maintenance	9 908 526
Insurance	1 651 421
G&A	461 500
Total fixed operating cost	12 731 947

7.5 Variable cost

Variable operating costs scale directly with plant throughput and are driven by the consumption of the ethane feedstock, process-side consumables and the utility envelope. They are evaluated on an annual basis at the base-year (2025) price level and are then escalated at 11.7%/year in the cash-flow model, consistent with the inflation assumption adopted in Chapter 7 introduction.

The raw-materials line is dominated by the ethane feedstock, which is consumed at 39,000 kg/h or roughly 297.2 kt/year at the contracted plant-gate price of \$80/t set out in Section 7.1. At a 64% per-pass conversion in the cracking furnaces, this feed supplies the 303.2 kt/year of polymer-grade ethylene product and the associated fuel-gas and C3+ by-product streams. On top of the feedstock, the raw-materials account absorbs the cost of process-side consumables, namely caustic for acid-gas and CO₂ removal, molecular-sieve desiccant in the dryer, amine make-up, corrosion inhibitors and the periodic replacement of the hydrogenation guard-bed catalyst. Extracting these items from Aspen Economics gives a combined base-year raw-material expenditure of \$63.67M per year, equivalent to 24.7% of the base-year revenue.

The utility envelope covers cooling water, imported electricity, fired-heater fuel, high- and low-pressure steam and the three mechanical-refrigeration stages (propane, propylene and ethylene cascade). Imported electricity is the single largest contributor at \$6.37M/year, driven by the 11.5 MW of compression duty across the cracked-gas and refrigeration compressor trains. Fired-heater fuel for the cracking furnaces adds \$3.12M/year at an inlet temperature of 1000 °C. The propylene and ethylene refrigerants together cost \$7.14M/year because of the very low-temperature duty required upstream of the C2-splitter, while cooling water together with HP and LP steam form a comparatively small group at \$4.07M/year combined. Summing the eight itemised utilities gives \$21.97M/year. The operating-cost model rounds this to the \$22.68M/year reported directly by Aspen Economics, which includes minor auxiliary natural-gas and instrument-air consumption that is not itemised in the utility summary. The full breakdown is given in Table 43.

Table 48. Utilities

Utility	Description	Annual Cost, US \$/yr
Cooling water	Process cooling water, 0.950 MMGAL/h	868 901
Electricity	Imported electrical utility, 11,455 kW	6 371 323
Fired heater fuel	Cracking furnace duty, 1000→400 °C	3 124 159
HP steam	High-pressure steam, 250 °C, 572 psia	1 258 664
LP steam	Low-pressure steam, 125 °C	1 947 415
Propane refrigerant	Refrigerant R2 (Propane), −40 °C	1 261 042
Propylene refrigerant	Refrigerant R3 (Propylene), −65 °C	3 991 236
Ethylene refrigerant	Refrigerant R4 (Ethylene), −103 °C	3 151 812
Total		21 974 551

Combining raw materials, utilities, fixed operating costs and the linear depreciation on the capital base gives the full operating-cost structure shown in Table 44. The environmental-fee line at 0.1% of revenue covers the CO₂ and other permit-based emission charges calculated from the Aspen emissions block and the disposal of the oily- and drain-water streams from the quench tower. Depreciation is booked on a straight-line basis over ten years on the sum of ISBL and OSBL (\$330.3M + \$66.1M = \$396.3M), which is discussed further in Section 7.6. The base-year total operating cost of \$138.92M is equivalent to 54.0% of the base-year revenue, leaving a margin of 46% before depreciation at the EBITDA level.

Table 49. Total operating cost breakdown

Cost Item	\$/yr	% of Revenue
Raw Materials	\$63 669 115	24.7%
Utility Cost	\$22 684 551	8.8%
Fixed Operating Costs (labor, maintenance)	\$12 731 947	4.9%
Environmental fee	\$205 279	0.1%
Depreciation	\$39 634 106	15.4%
Total Operating Costs	\$138 924 997	54.0%

7.6 Economic analysis

Combined cost of production (CCOP) is defined as the sum of variable and fixed operating costs:

$$CCOP = VCOP + FCOP \quad (26)$$

The value of CCOP or total operating costs is \$138.9M per year. The gross profit is calculated by subtracting the CCOP from the Revenue. The depreciation was considered as linear over 10-year span on the sum of total installed cost (TIC) and support facilities (OSBL)

$$D = \frac{TIC + OSBL}{10} = \frac{330,284,214 + 66,056,843}{10} = \$39,634,106/\text{year}$$

$$R_0 = 303245 \cdot \$844 + 5185 \cdot \$50 + 8208 \cdot \$150 = \$287,548,498/\text{year}$$

R_0 is the base-year revenue from the three products, which is inflated by the 11.7%/year rate annually. Due to SEZ, the corporate income tax, VAT on imports, property tax are equal to 0% and free-customs-zone regime, leading to no taxation assumptions [99].

Table 45 provides net and cumulative cash flows for each 2 years over the span of a decade . Adjusted cash flow is calculated considering the operating expenses, depreciation and waste treatment processes. The full prospect of cash flows are shown in Figure 18.

Table 50. Net and cumulative cash flows

Year	2028	2030	2032	2034	2036	2038
------	------	------	------	------	------	------

Net Cash Flow	\$ (216,7M)	\$ 176,6M	\$ 220,4M	\$ 274,9M	\$ 343,1M	\$ 428.1M
Cumulative Cash Flow	\$ (216,7M)	\$ (374,9M)	\$ 42,8M	\$ 563,9M	\$ 1,214.2M	\$ 2,025.5M

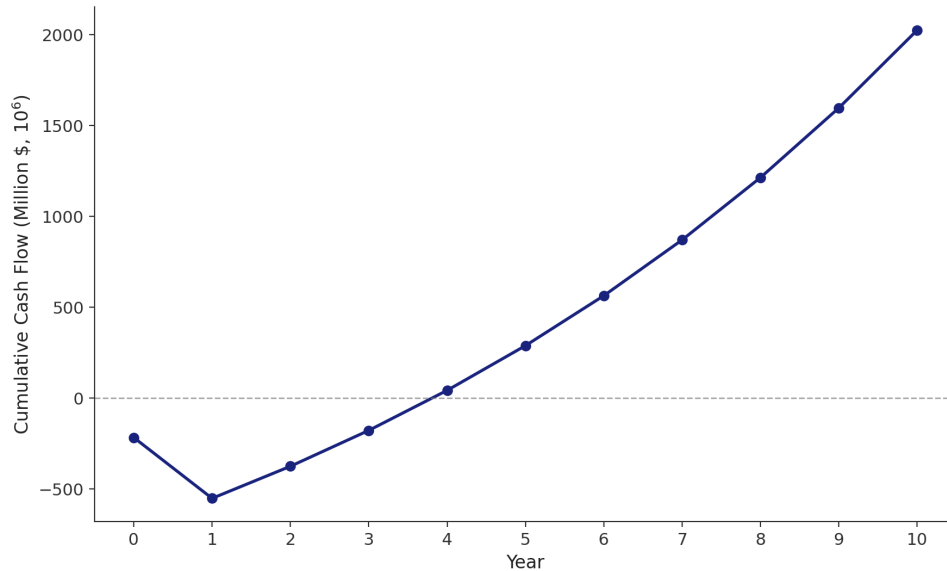


Figure 18. Cumulative cash flow for 10 years

This table shows the project cash flow profile over the construction and operating periods. The plant experiences large negative cash flows during the construction years due to capital investment and working capital requirements, with the lowest cumulative cash flow reached before start-up. Once operations begin, annual net cash flow becomes positive and grows over time due to inflation-adjusted revenues. The cumulative cash flow turns positive in 2032, which confirms that the project recovers its investment in the fifth year of its operation. If more precisely:

$$\text{Payback} = 2 \text{ yr construction} + 1 + \frac{177626547 + 42765951}{177,626,547} = 4.24 \text{ years from 2028}$$

Therefore, the table demonstrates that although the plant is highly capital-intensive at the beginning, it generates strong cash returns after start-up.

From the annual cash flow at the 20% weighted average cost of capital, the net present value or investment profitability can be calculated:

$$NPV = \sum_{t=0}^{10} PV_t = \sum_{t=0}^{10} \frac{CF_t}{(1+i)^t} = \$459,758,594 \quad (27)$$

Internal rate of return is 34.6%, while profitability index is 1.69, meaning every dollar invested returns \$1.69 of present-value net cash. Return on investment on an average net profit basis is $222.03 / 502.03 = 44\%$ in the base year.

Table 51. Financial summary of the plant key metrics

Finance Summary		
Metric	Value	Note
Net Present Value (NPV)	\$347 315 525	The total value created by the project in today's dollars
Internal Rate of Return (IRR)	34.6%	The actual return rate the project generates on invested capital
Simple Payback (years)	4	The years are required to payback from base year
Profitability Index	1.69	$(NPV + Investment) / Investment$
Total Revenue (Base)	\$257 429 273	The annual revenue at base year prices before inflation.
Total OpEx (Base)	\$138 924 997	Total annual operating costs at base year prices
Earnings Before Interest, Tax, Depreciation and Amortisation	66.5%	The project is marginally profitable at the operating level

Chapter 8. Conclusions and Future Work

Project overview

This capstone project has delivered the complete detailed-engineering design of a 300 kt/y polymer-grade ethylene plant based on ethane steam cracking, to be located in Atyrau, Kazakhstan. Across Reports 1 – 4 the project progressed from feedstock and market analysis (Report 1), through process-route selection and mass-and-energy balance (Report 2), to the Aspen Plus simulation and preliminary equipment sizing (Report 3), and finally to the detailed design of every major and minor unit, the plant layout and the economic evaluation in Report 4. The whole package meets the 99.95 mol % ethylene product specification and the 5 ppm acetylene ceiling required for polymer-grade service, and uses an ethane feed that is fully available from the Tengiz and Kashagan gas streams.

Process route and mass-and-energy balance

Ethane steam cracking was selected over alternative routes (naphtha cracking, methanol-to-olefins, ethanol dehydration) because of the high ethylene selectivity (~80 %), the ready local availability of ethane from the Tengiz and Kashagan gas-liquids fractionation, and the favourable CO₂ footprint relative to naphtha cracking. The Aspen Plus v12 simulation (RK-SOAVE equation of state) closed a 17,050 kg/h ethane feed with a 31 % steam-to-ethane ratio at the furnace inlet, yielding 35,941 kg/h of polymer-grade ethylene, 1,044,000 kg/h of quench-water circulation and a full cold-box separation train. Chapter 2 summarises the plant-wide material and energy balance and establishes the feed rates, duties and operating conditions carried forward into Chapter 3.

Major equipment design

R-101. The pyrolysis furnace operates at 850 °C coil outlet with a tube-wall temperature of 1050 – 1100 °C. HP40-Nb alloy (35 % Ni, 25 % Cr, 1.5 % Nb, Fe balance) was selected over HK40 and HP40 because the niobium addition stabilises the carbide microstructure during thermal cycling, suppresses σ -embrittlement and pushes the design life beyond 5 years. A parametric sweep (1 – 80 tubes) fixed the configuration at 77 tubes of 6" schedule-40, 4.5 m length, giving a pressure drop of ~2,000 Pa and inlet/outlet velocities of 15 / 40 m/s. Wall-thickness verification with the ASME VIII Div. 1 hoop-stress relation and a 5-year corrosion allowance confirmed the schedule-40 selection.

E-104. E-104 recovers heat from the 820 °C cracked-gas effluent against the 450 °C feed to the furnace. LMTD / F-factor sizing (Appendix D) and a Kern / Dittus-Boelter overall heat-transfer coefficient of 571 W/(m²·K) resulted in a 175 m² shell-and-tube exchanger with 532 tubes on six passes, a 0.143 bar shell-side pressure drop and a 0.123 bar tube-side drop, both comfortably below the design ceilings.

T-104. The cryogenic demethaniser sits at –98 °C / 33 bar on the top tray and separates methane and hydrogen from the C₂+ cracked-gas stream. FUG shortcut combined with a rigorous RadFrac simulation fixed the column at 35 theoretical stages with the feed on stage 21, a reflux ratio of $1.6 \times R_{\min}$, and a condenser duty of 32 MW against propylene refrigerant. The design meets a methane-in-ethylene specification of < 100 ppm and recovers > 99.5 % of the C₂+ inventory.

R-102 / R-103. The individual-student design of the AHU (reported in this document, Chapter 3 in full and Appendices A – E in detail) delivered a two-stage adiabatic packed-bed arrangement with staged H₂ injection on a Pd-Ag / γ -Al₂O₃ catalyst. The unit meets the polymer-grade 27.5 ppm acetylene outlet specification — a 5 $\times$ margin on the 5 ppm ceiling — while maintaining ethylene selectivity above 70 %, a maximum bed temperature of 63.1 °C (well below the 85 °C

Pd-sintering threshold), and a combined pressure drop of 0.21 bar against a 0.5 bar design ceiling.

T-106. The superfractionator separates ethylene from ethane at 9 bar / $-30\text{ }^{\circ}\text{C}$. A Fenske-Underwood-Gilliland shortcut gave ~ 120 theoretical stages with a reflux ratio of $4.2 \times R_{\min}$, validated against a RadFrac rigorous simulation. The column produces 99.95 mol % ethylene overhead and recycles the ethane bottoms back to the furnace feed header to suppress greenfield ethane make-up.

Minor equipment design

Chapter 4 consolidated the full minor-equipment schedule: seven shell-and-tube / plate-fin heat exchangers (E-101 – E-107) sized against Sinnott and Perry heuristics with Incoloy 800HT for high-temperature service to suppress carburisation; the three-stage cracked-gas compression train C-101 / C-102 / C-103 sized following Corbò pressure-ratio and inter-cooling rules to a 38 bar discharge; the quench tower T-101 sized with the KLM energy-balance procedure; the zeolite-3A molecular-sieve dryer T-102 sized for a < 1 ppm water specification ; the cryogenic hydrogen separator T-103; the static mixer M-101; the full plant valve catalogue drawn from the six HAZOP nodes; and the four storage tanks TK-101 – TK-104 (ethylene product, ethane feed, propylene refrigerant, quench-water surge). Storage-tank design follows API 625 for cryogenic full-containment service and API 620 Annex Q for low-temperature containment; PSV sizing on every protected vessel follows API 520 and vessel shells follow ASME VIII Div. 1 .

Plant location and layout

The Atyrau petrochemical zone was chosen on the basis of feedstock proximity (direct pipeline access to the Tengiz and Kashagan gas-liquids fractionation), Caspian port access for product export, and an existing workforce with petrochemical experience. The plot-plan respects API 752 and NFPA 30 separation distances between the cracking furnace fire-box, the compression bay, the cold-box area and the storage-tank farm. Prevailing-wind and topography considerations place the flare stack downwind of the process area and the storage-tank farm bunded at 110 % containment per API 625.

Process-safety and HAZOP

A six-node HAZOP was completed across the full plant: N1 ethane feed, N2 cracking furnace, N3 quench and compression, N4 drying and hydrogen separation, N5 demethaniser / C2 splitter, and N6 hydrogenation. Node 6 (AHU) is reproduced in full in Appendix G together with the consolidated valve-action catalogue. Two SIL-2 deviations were identified on the AHU (H6.3 excess H_2 injection and H6.5 reactor over-pressure) and are protected by a TAAH 2003

bed-thermocouple interlock, a FAHH hydrogen-flow interlock, and a PSV sized for the API 520 fire case. Every compressor stage is protected against surge, and every distillation column is protected against reboiler runaway by a fail-closed TCV on the steam supply.

Economic analysis

Future work

The following follow-up activities are identified for subsequent revisions of the plant design:

1. **Three-feed-stage separator configuration.** Investigate a modified separator configuration in which the cracked-gas stream is introduced at three different stages instead of a single feed point. Splitting the feed across the column height equalises the internal pressure profile, reduces the hydraulic step-change at the feed stage, and smooths the vapour-load / liquid-load distribution across the rectifying and stripping sections. This is expected to reduce the reflux duty, flatten the temperature gradient, and lower the risk of local flooding or weeping in the feed-zone trays.
2. **Alternative lead / guard-bed configurations for the AHU.** Explore alternative lead-bed / guard-bed arrangements — for example three beds in series with mid-bed H₂ re-injection, a swing configuration in which any of three beds can be rotated into the lead position, or a radial-flow packed-bed geometry — with the objective of extending the catalyst-rotation interval beyond the baseline 360 days and pushing the overall catalyst service life beyond the current 8-year ceiling before Pd-sintering-driven replacement.
3. **Alternative AHU catalyst formulations.** Bench-mark the baseline Pd-Ag / γ -Al₂O₃ catalyst against newer formulations — Pd-Au / Al₂O₃, Ni-based non-precious-metal catalysts, bimetallic Pd-Cu, and Pd-Ga intermetallics — in order to generate a side-by-side comparison of LHHW kinetic parameters, selectivity-versus-conversion envelopes, deactivation time-constants, and full-life economics. The outcome is a recommendation on whether catalyst substitution would improve either the kinetic performance or the OpEx footprint of the hydrogenation unit.
4. **Naphtha-cracking comparative study.** Build a full mirrored design for a naphtha-cracking plant of equivalent ethylene capacity and benchmark it against the current ethane-based design on both technical grounds (ethylene yield, by-product slate including propylene / butadiene / aromatics, energy intensity, CO₂ footprint, feedstock flexibility) and economic grounds (CapEx, OpEx, NPV, IRR, sensitivity to crude-oil price versus natural-gas-liquids price). The comparison will establish which route is more technically feasible and economically effective for the Kazakhstan market.
5. **3D plant layout.** Develop a 3D plot plan and piping general-arrangement model of the full plant — cracking furnace F-101, feed-effluent exchanger E-104, AHU R-102 / R-103 pair, demethaniser T-104, C2 splitter T-106, compression bay, cold box and storage-tank farm — in a dedicated 3D CAD / plant-design package, respecting API 752 and NFPA 30 separation

distances and generating clash-free equipment spacing, access routes and piping trays ready for detailed-engineering hand-over.

Closing remarks

Reports 1 through 4 taken together deliver the complete process-engineering package for a 300 kt/y polymer-grade ethylene plant at Atyrau, Kazakhstan. The plant meets every product-quality and process-safety target set out in Report 1, is technically feasible on the basis of the Aspen Plus mass-and-energy balance validated in Report 3, and the detailed equipment design documented in Chapters 3 – 5 of this report is consistent with the applicable API, ASME, TEMA and IEC codes. With the economic module to follow, the design package will be ready for front-end loading (FEL-3) hand-over to a detailed-engineering contractor and is positioned to make a meaningful contribution to the downstream development of Kazakhstan's petrochemical sector.

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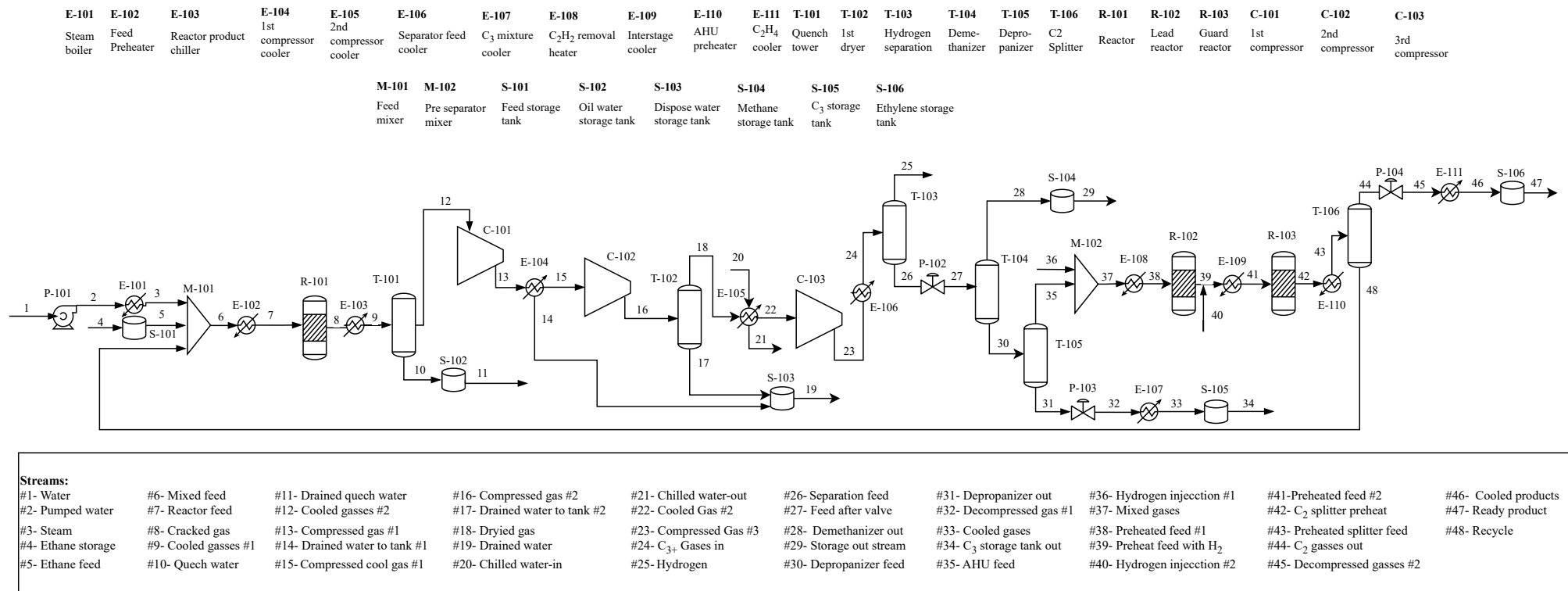
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List of Appendices

Appendix A. Reaction Kinetics

Contains the reaction network and kinetic parameters used to model the chemical reactions in the system.

Appendix B. Reactor Sizing Calculations

Presents detailed calculations for reactor design, including mass balances, ideal gas relations, pressure drop estimation, tube selection, and reactor dimensions.

Appendix C. Material Selection for Reactor

Explains the selection of construction materials for the reactor based on high-temperature performance, creep resistance, and resistance to carbon deposition.

Appendix D. Heat Exchanger Calculations

Includes thermal design calculations such as heat duty, LMTD, heat transfer coefficients, required surface area, and pressure drop for the heat exchangers.

Appendix E. Acetylene Hydrogenation Kinetics

Describes the kinetic model (LHHW) for acetylene hydrogenation, including rate expressions, parameter values, reactor performance, and validation data.

Appendix F. Storage Tank Sizing Calculations

Provides sizing methodology and results for storage tanks based on process flow rates, holding times, safety factors, and industry standards.

Appendix G. Equipment List and Cost Estimation

Lists major process equipment along with cost estimates, installation factors, and total installed costs for economic evaluation.

Appendix A. Reaction Kinetics

Table A1. Reaction Network and Kinetics.

No	Reaction	$A, \frac{1}{sec}$	E, kcal/mole
1	$C_3H_8 \Rightarrow^{k_1} C_2H_4 + CH_4$	$4.692 \cdot 10^{10}$	50.60
2	$C_3H_8 \Rightarrow^{k_2} C_3H_6 + H_2$	$5.888 \cdot 10^{10}$	51.29
6	$C_3H_6 \Leftrightarrow^{k_6} C_2H_2 + CH_4$	$3.794 \cdot 10^{11}$	59.39
6'	$C_2H_2 + CH_4 \Rightarrow^{k_{6'}} C_3H_6$	$2.33 \cdot 10^7$	29.6
8	$C_2H_6 \Leftrightarrow^{k_8} C_2H_4 + H_2$	$4.652 \cdot 10^{13}$	65.20
8'	$C_2H_4 + H_2 \Rightarrow^{k_{8'}} C_2H_6$	$9.89 \cdot 10^8$	33.0

Appendix B. Reactor sizing calculations

$$\frac{dF_j}{dV} = r_j \quad (\text{B1})$$

where,

F_j - molar flow rate, kmol/h

r_j - net rate of generation, kmol/(m³*h)

V - volume, m³

$$\begin{aligned} \frac{dF_{C_2H_6}}{dV} &= -r_8 \\ \frac{dF_{C_2H_4}}{dV} &= r_1 + r_8 \\ \frac{dF_{H_2}}{dV} &= r_2 + r_8 \\ \frac{dF_{CH_4}}{dV} &= r_1 + r_6 \\ \frac{dF_{C_3H_6}}{dV} &= r_2 - r_6 \\ \frac{dF_{C_3H_8}}{dV} &= -r_1 - r_2 \\ \frac{dF_{C_2H_2}}{dV} &= r_6 \end{aligned}$$

The concentrations at each integration step are calculated from the ideal gas law at 2 bars by equations (2)

and (3).

$$C_T = \frac{P}{R^*T} \quad (\text{B2})$$

where,

C_T - total molar concentration, kmol/m³

P - pressure in the reactor, 2 bar

R - universal gas constant, 0.08314 bar*m³/(kmol*K)

T - temperature in the reactor, 1123.15 K

$$C_j = \frac{F_j}{F_T} * C_T \quad (\text{B3})$$

where,

C_j - molar concentration for each species, kmol/m³

F_T - total molar flow rate, kmol/h

The corresponding ODEs were solved in Python using Euler Method, integration proceeded in volume steps of $\Delta V=0.0001$ m³ until target conversion was reached. The step size is verified by the fact that changing it to half changed the final volume by just 0.1%.

Pressure drop along the length of the tubes was calculated using Haaland correlation for Darcy friction factor, in turbulent flow regime.

$$\frac{1}{\sqrt{f}} = -1.8 * \log_{10} \left[\left(\frac{\varepsilon}{D} \right)^{3.7} + \frac{6.9}{Re} \right] \quad (B4)$$

where,

f - darcy friction factor

ε - surface roughness, m

D - diameter of the tube, m

Re - Reynolds number

The number of tubes were adjusted based on the velocity and pressure drop, to achieve the reasonable values different arrangements were calculated. To balance both the number of tubes and tube diameter outer diameter of 6 inch schedule 80 tubes were initially chosen [1].

Further it was calculated that we can use tubes with thinner walls by equation (5). The value for allowable stress was used for 982°C for the HP40-Nb alloy[3].

$$Sch = \frac{P}{\sigma} * 1000 = \frac{0.2 MPa}{17.3 MPa} * 1000 = 11.56 \quad (B5)$$

where,

Sch - schedule of the tube

P - pressure inside the tube, MPa

σ - allowable stress for chosen material, MPa

Even though the calculated Schedule is 12, I take Schedule 40 tubes since the data available only for schedule 40 and 80 tubes.

A parametric study was conducted varying the number of tubes from 1 to 80, with Schedule 80 6 inch outer diameter tubes 80 tubes with length of 4.8 m (around 16 feet) was chosen, however after changing the tubes to Schedule 40 6 inch outer diameter, 77 tubes of length approximately 4.5 m (corresponding to 15 feet) was chosen. This configuration allowed a reasonable pressure drop of around 2000 Pa, and velocity of the fluid 15 and 40 m/s on the inlet and outlet, respectively. The comparison table is depicted in the excel sheet.

Based on the tube inside diameter, corrosion rate, allowable stress, weld strength reduction factor, coefficient of material used, and weld quality factor the wall thickness was calculated with the equation (6).

$$t = \frac{PD}{2*(SEW+PY)} + C \quad (B6)$$

where,

t - wall thickness

P - pressure inside the tube, MPa

D - tube outside diameter, mm

C - corrosion rate, mm

S - allowable stress, MPa

E - weld quality factor, 1.0

W - weld strength reduction factor, 1.0

Y - coefficient of materials used, 0.7

The wall thickness calculated considering the corrosion for 5 years is 2.46 mm, which is more than covered by 6 inch schedule 40.

The height of the reactor consists of the length of the individual tube 4.57 m (15 feet) + clearance height of 2m.

Appendix C. Material Selection for reactor

With the process gas at 850°C, the tube wall temperature is estimated to be 1050-1100°C, at this thermal environment and carbon-rich atmosphere three austenitic alloys are commonly used for pyrolysis furnace tubes [2]:

HK40 (25% Ni, 25% Cr, Fe balance) - previous industry standard, with combination of lower manufacturing costs and satisfactory mechanical properties up to 1000°C, but it has problems with carbon deposition and lower creep resistance, compared with higher nickel alloys.

HP40 (35% Ni, 25% Cr, Fe balance) - widely used for newer installations, higher nickel content increases resistance to carbon deposition and creep strength.

HP-40-Nb (35% Ni, 25% Cr, 1.5% Nb, Fe balance) - the addition of niobium creates additional thermal stability by stabilizing the carbide microstructures during multiple heating cycles, further improving high-temperature creep strength.

As a result HP-40-Nb was selected for R-101. The niobium addition plays an important role of suppressing sigma embrittlement and improves long-term creep performance; it yields a design life of more than 5 years.

Appendix D. Heat Exchanger calculations

The calculations for the heat exchangers design is provided in the following equations:

1. Heat duties and Cold water flow rate

$$Q = mC_p \Delta T \quad (D1)$$

$$Q = 17.05 * 2.454 * (81.66 - 33) = 2035.96$$

$$2035.96 = m * 4.52 * (35 - 20)$$

$$m=30.03 \text{ kg/s of water for Heat exchanger}$$

2. The next part is to calculate LMTD for the process, together with correction factor:

$$Q = \frac{\Delta T_1 - \Delta T_2}{\ln(\frac{\Delta T_1}{\Delta T_2})} = \frac{46.66 - 13}{\ln(\frac{46.66}{13})} = 26.34^\circ \text{C}$$

$$R = \frac{T_{h \text{ in}} - T_{h \text{ out}}}{T_{c \text{ in}} - T_{c \text{ out}}}$$

$$S = \frac{T_{c \text{ out}} - T_{c \text{ in}}}{T_{h \text{ in}} - T_{c \text{ in}}}$$

$$F = \frac{\sqrt{R^2 + 1}}{R - 1} * \frac{\ln(\frac{1-S}{1-RS})}{\ln(\frac{2/S - 1 - R + \sqrt{R^2 + 1}}{2/S - 1 - R - \sqrt{R^2 + 1}})}$$

$$\Delta T_{lm} = F * \Delta T_{lm,cf}$$

3. Preliminary overall coefficient and required area

$$UA = \frac{Q}{\Delta T_{lm}} = \frac{2036.3}{20} = 101.8 \text{ kW/K} \quad (D2)$$

$$F = \frac{UA}{U_d} = \frac{101.8}{0.58} = 175.5 \text{ m}^2 \quad (D3)$$

4. Tube side geometry and flow calculations

Area per tube:

$$A_t = \pi i * D_o L = 3.14 * 0.025 * 4.2 = 0.3297 \text{ m}^2 \quad (D4)$$

Number of tubes:

$$N_t = \frac{A_{req}}{A_t} = 532 \quad (D5)$$

Tube per passes

$$N_{t/p} = \frac{N_t}{n_p} = \frac{532}{6} = 89 \quad (D6)$$

Total tube-side flow area:

$$A_{c,t} = \frac{\pi i^2 D_i^2}{4} \frac{N_t}{n_p} = 0.03278 \text{ m}^2 \quad (D7)$$

Cold water velocity:

$$u_c = \frac{m_c}{\rho_c A_c} = 0.9 \text{ m/s} \quad (\text{D8})$$

Reynolds number (tube-side):

$$Re_t = \frac{\rho_c * u_c * Di}{\mu_c} = 22340 \quad (\text{D9})$$

Prandtl number (tube side)

$$Pr_t = \frac{C_{p,c} * \mu_c}{k_c} = 6.54 \quad (\text{D10})$$

Nusselt number (tube side):

$$Nu_t = 0.023 Re_t^{0.8} * Pr_t^{0.4} = 147 \quad (\text{D11})$$

Cold water velocity:

$$h_i = \frac{Nu_t * k_c}{Di} = 4171.7975 \quad (\text{D12})$$

Pitch

$$p_t = 1.25 * Di = 0.03125 \quad (\text{D13})$$

5. Shell side calculations

Shell diameter

$$D_s = p_t * 1.13 \sqrt{N_t} + 0.038 = 0.689 \text{ m} \quad (\text{D14})$$

Number of baffles

$$N_b = \frac{L}{B} - 1 = 26 \quad (\text{D15})$$

Cross-flow area at the shell centre

$$A_s = \frac{pi}{4} * D_s^2 - N_t \frac{pi}{4} D_o^2 = 0.112 \text{ m} \quad (\text{D16})$$

Mass velocity (shell side):

$$G_s = \frac{m_h}{A_s} = 152 \text{ kg/s} * \text{m}^2 \quad (\text{D17})$$

Equivalent diameter for square pitch:

$$d_e = \frac{4(p_t^2 - \frac{pi}{4} D_o^2)}{pi * D_o} = 0.0068 \text{ m} \quad (\text{D18})$$

Shell-side Re number:

$$Re_s = \frac{G_s * d_e}{\mu_h} = 73541 \quad (\text{D19})$$

Shell-side Pr number:

$$Pr_s = \frac{C_{p,h} \mu_h}{k_h} = 0.6277 \quad (D20)$$

Shell-side heat transfer coefficient (Dittus-Boelter type correlation):

$$h_o = 0.036 * \left(\frac{k_h}{d_e}\right) Re_s^{0.8} * Pr_s^{1/3} = 1947 \text{ W/m}^2 \quad (D21)$$

6. Overall heat transfer coefficient

Shell-side film resistance

$$R_{film} = \frac{1}{h_o} = 0.000513367 \text{ m}^2 * K/W \quad (D22)$$

Shell-side fouling:

$$R_{film} = 0.0002 \text{ m}^2 * K/W \quad (D23)$$

Tube wall resistance:

$$R_{film} = \frac{Do * \ln(Do/Di)}{2 * k_w} = 3.93E - 05 \text{ m}^2 * K/W \quad (D24)$$

Tube-side film resistance

$$R_{film} = \frac{1}{h_i} * \frac{D_o}{D_i} = 0.000239705 \text{ m}^2 * K/W \quad (D25)$$

Tube-side fouling resistance

$$R_{film} = 0.0006 * \frac{D_o}{D_i} = 0.000691 \text{ m}^2 * K/W \quad (D26)$$

Total thermal resistance

$$\frac{1}{U_o} = R_{film,o} + R_{f,o} + R_w + R_{film,i} + R_{f,i} = 0.00172 \quad (D27)$$

$$U_o = 571 \text{ W/m}^2 * K$$

7. Pressure drop calculations

Shell-side:

$$\Delta P_s = 1.3 * 4 * f_s * \frac{L}{d_e} * \left(0.5 \frac{G_s^2}{\rho_h}\right) = 14329.7 \text{ Pa} = 0.143297 \text{ bar} \quad (D28)$$

Tube-side:

$$\Delta P_t = 4 * f_t * \frac{L}{d_i} * (0.5 * \rho_c * u_c^2) + 4 * 2.5 * (0.5 * \rho_c * u_c^2) = 12347.21 \text{ Pa} = 0.123 \text{ bar}$$

Appendix E. Acetylene hydrogenation kinetics

Acetylene hydrogenation on Pd-Ag/Al₂O₃ is represented using a LHHW rate expression. The model captures competitive adsorption of hydrogen, acetylene, and ethylene, including inhibition by the high ethylene partial pressure in the C₂-rich stream.

Rate expression for acetylene consumption

$$r_1 = \frac{k_4 K_1 K_2 P(C_2H_2) P(H_2)}{[1 + \sqrt{(K_1 P(H_2)) + K_2 P(C_2H_2) + P(C_2H_4)/K_5}]^2} \quad (E1)$$

At 333 K (60 °C), the parameter values adopted for validation are listed in Table E1. Under the selected tail-end operating conditions, the ethylene inhibition term is expected to dominate the denominator, which supports high selectivity by suppressing over-hydrogenation.

Table E1. Kinetic and physical parameters

Parameter	Symbol	Value	Units
Acetylene rate constant	k ₄	5.26 x 10 ⁻³	mol/(kg·s)
Hydrogen adsorption constant	K ₁	13.00	bar ⁻¹
Acetylene adsorption constant	K ₂	107.00	bar ⁻¹
Ethylene inhibition constant	K ₅	7.40	bar
Catalyst bulk density	ρ _{bulk}	720.00	kg/m ³
Bed void fraction	ε	0.40	-
Mixture heat capacity (validation basis)	C _{p,mix}	55.00	J/(mol·K)

The LHHW expression was evaluated at the Reactor 1 (R-1) inlet conditions (333 K, 25 bar) to obtain the maximum local rate. The observed reactor-average rate is lower because acetylene concentration decreases continuously along the bed. The average rate is therefore defined by catalyst-mass integration of the local rate expression.

Average-rate definition over the R-1 catalyst bed

$$r_{avg, R-1} = (1/W_1) \int_0^{W_1} r_1 dW \quad (E2)$$

Inlet-to-average rate comparison ratio

$$\phi_{R-1} = r_{1, inlet} / r_{avg, R-1} \quad (E3)$$

Table E2. Kinetic validation summary for R-1.

Metric	Value
Calculated inlet rate, r _{1,inlet}	1.47 x 10 ⁻⁴ mol/(kg·s)

Observed average rate, $r_{avg,R-1}$	$8.62 \times 10^{-5} \text{ mol}/(\text{kg}\cdot\text{s})$
Inlet/average ratio, Φ_{R-1}	1.70

Both AHU reactors are treated as adiabatic packed-bed plug flow reactors with identical vessel diameter. Catalyst-bed geometry is obtained from catalyst mass, bulk density, and selected vessel diameter. Only the governing sizing relationships are shown below.

Catalyst-bed volume from catalyst inventory

$$V_i = W_i / \rho_{bulk} \quad (E4)$$

Reactor cross-sectional area

$$A = \pi D^2 / 4 \quad (E5)$$

Bed height

$$L_i = V_i / A \quad (E6)$$

Bed aspect ratio criterion

$$(L/D)_i = L_i / D \quad (E7)$$

Table E3. AHU reactor performance and geometry summary

Parameter	R-1 (Lead bed)	R-2 (Guard bed)	Units
Inlet temperature	60.0	63.1	°C
Outlet temperature	63.1	62.1	°C
Pressure	25	25	bar
C2H2 inlet	572	247	ppm
C2H2 outlet	247	27.5	ppm
Acetylene conversion	56.9	88.9	%
Catalyst mass	2100	5000	kg
Vessel diameter	1.9	1.9	m
Bed length	1.029	2.449	m
Ergun pressure drop	0.062	0.148	bar

Space velocity and contact time are reported using actual volumetric flow rates at operating conditions from Aspen Plus. These relations are used to compare the lead bed and guard bed contact severity.

Gas hourly space velocity

$$GHSV_i = Q_i / V_i$$

Empty-bed contact time for each bed

$$EBCT_i = V_i / Q_i$$

Combined empty-bed contact time

$$EBCT_{total} = EBCT_{R-1} + EBCT_{R-2}$$

Interstitial gas residence time

$$t_{interstitial} = \varepsilon \cdot EBCT_{total}$$

Table E4. Space velocity and contact-time summary.

Metric	R-1	R-2	Units
GHSV	659	280	h ⁻¹
EBCT	5.46	12.84	s
Combined EBCT	18.30	-	s (R-1 + R-2)
Interstitial residence time	7.3	-	s (combined)

The adiabatic temperature rise in R-1 is estimated using the total heat released by the desired acetylene hydrogenation reaction and the undesired ethylene hydrogenation reaction. A constant mixture heat capacity is used for the hand calculation, and Aspen Plus is used as the reference for final validation.

Total reaction heat release

$$Q_{reaction} = \sum [(-\Delta H^{\circ}) \cdot n, consumed]$$

Adiabatic temperature rise

$$\Delta T_{rise} = \frac{Q_{reaction}}{n_{mix} C_p}$$

Table E5. Adiabatic temperature-rise validation summary for R-1.

Quantity	Value
Predicted adiabatic temperature rise (hand calculation)	3.24 °C
Aspen temperature rise (HEAT stream)	3.14 °C
Agreement	Within 3%

Hydrogen injection is staged to maintain a controlled H₂/C₂H₂ ratio in each reactor. This avoids hydrogen starvation in the lead bed while limiting excess hydrogen in the guard bed, thereby preserving selectivity to ethylene.

Stage inlet hydrogen-to-acetylene molar ratio

$$\frac{R_{H_2}}{C_2H_2} = \frac{n_{H_2}}{n_{C_2H_2}}$$

Table E6. Selected stage inlet H₂/C₂H₂ ratios and interpretation.

Stage	Selected ratio
R-1 (Lead bed)	2.89
R-2 (Guard bed)	1.32

Appendix F. Storage-tank sizing calculations

Four dedicated storage tanks (TK-101 through TK-104) serve the plant: ethylene product, ethane feed, propylene refrigerant, and a quench-water surge drum. All tanks are sized from the Chapter 3 Aspen mass-flow data with an ullage factor of 0.85 (15 % vapour space per API 625 for cryogenic service [42]) and a 10 % engineering safety margin on the net volume [6]. Industry-standard holding times are used [6, 10]: 3 days downstream-buffer for ethylene product, 5 days feedstock security for ethane, 7 days for propylene refrigerant inventory plus spare, and 30 min surge for quench water.

Table F.1. Storage-tank sizing basis.

Parameter	Value	Source / basis
Plant operating hours	8,000 h/yr	Continuous olefins plant
Ethylene production rate	1,281.35 kmol/h	T-103 bottoms (Aspen)
Ethylene mass flow	35,941 kg/h	MW 28.05 kg/kmol
Ethane fresh feed	900 kmol/h	Industry typical ethane cracker
Ethane mass flow	27,063 kg/h	MW 30.07 kg/kmol
Quench water circulation	1,044,000 kg/h	Quench-tower energy balance
Liquid ethylene density (−104 °C)	567 kg/m ³	Perry's Handbook [25]
Liquid ethane density (−89 °C)	544 kg/m ³	Perry's Handbook [25]
Liquid propylene density (−47 °C)	609 kg/m ³	Perry's Handbook [25]
Ullage factor	0.85	15 % vapour (API 625) [42]
Design margin	1.15	10 % engineering margin [6]

Table F.2. Storage-tank sizing results.

Tag	Service	Fluid / T	Hold	Mass to store (t)	Net V (m ³)	Recommended size
TK-101	Ethylene product	Liq. C ₂ H ₄ / −104 °C	3 d	2,588	4,562	6,500 m ³ (2 × 3,250, API 625)
TK-102	Ethane feed	Liq. C ₂ H ₆ / −89 °C	5 d	3,248	5,970	9,000 m ³ (2 × 4,500, API 620 Q)

Tag	Service	Fluid / T	Hold	Mass to store (t)	Net V (m ³)	Recommended size
TK-103	Propylene refrigerant	Liq. C ₃ H ₆ / −47 °C	7 d	1,414	2,321	3,500 m ³ (API 620 Q)
TK-104	Quench water surge	Water / 35–82 °C	30 min	522	522	750 m ³ (CS drum)

All cryogenic tanks are full-containment, insulated with polyurethane foam between the inner 9 % Ni steel shell and the outer carbon-steel containment, per API 625 [42]. Boil-off gas (BOG) from TK-101 and TK-102 is recovered to the fuel-gas header via a small 1.5 MW BOG re-compressor [42, 43]. TK-103 and TK-104 are atmospheric with a blanket-gas system (nitrogen) to keep the vapour space inert [43].

Appendix G. Equipment list with factors, equipment cost and installation cost

Equipment	Name	Equipment Cost (USD)	Installation Factor	Material Factor	Installation Cost	Size reference	Unit
C-101	compressor 1	\$10,057,100	2.50	1.00x	\$48,106,462		
C-102		\$1,817,300	2.50	1.10x	\$9,562,027		
C-103		\$1,843,000	2.50	1.30x	\$11,460,388		
E-101	feed preheater	\$230,200	3.50	1.30x	\$2,004,044	15819.10x	kW
E-102	heater	\$397,191	3.50	1.50x	\$3,989,779	39264.90x	kW
E-103	cooler	\$3,231,800	3.50	1.30x	\$28,134,976	-38414.34x	kW
E-104		\$262,700	3.50	1.30x	\$2,286,979		
E-105		\$191,800	3.50	1.30x	\$1,669,747		
E-107	cooler before the storage	\$168,100	3.50	1.30x	\$1,463,423		
E-108		\$113,600	3.50	1.00x	\$760,741		
E-109		\$81,900	3.50	1.00x	\$548,457		
E-110	cooler before c2 splitter	\$1,293,437	3.50	1.30x	\$11,260,230	-8349.52x	kW
E-111	cooler after c2 splitter	\$469,200	3.50	1.30x	\$4,084,699	-1540.57x	kW
P-101		\$72,100	4.00	1.00x	\$551,805		
R-101	Main reactor	\$8,560,000	2.00	1.70x	\$55,685,653		
R-102	AHU 1	\$110,400	2.00	1.30x	\$549,203		
R-103	AHU 2	\$276,100	2.00	1.30x	\$1,373,505		
S-101	Feed Storage Tank	\$5,466,667	4.00	1.00x	\$30,613,333		
S-102	Oily Water Tank	\$157,167	4.00	1.00x	\$1,202,849		
S-103	Drain Water Tank	\$157,167	4.00	1.00x	\$1,202,849		

S-104	Methane Storage Tank	\$1,038,667	4.00	1.00x	\$7,949,262		
S-105	C3+ gases Storage Tank	\$116,167	4.00	1.00x	\$889,062		
S-106	Ethylene Storage Tank	\$4,100,000	4.00	1.00x	\$31,378,667		
T-101	Quench Tower	\$600,500	4.00	1.30x	\$5,974,575		
T-102	Dryer	\$204,900	4.00	1.30x	\$2,038,618		
T-103	Hydrogen Separation	\$277,900	4.00	1.30x	\$2,764,920		
T-104	Demethanizer	\$1,363,400	4.00	1.30x	\$9,925,552		
T-105	Depropanizer	\$5,691,200	4.00	1.00x	\$31,870,720		
T-106	C2-splitter	\$2,882,100	4.00	1.30x	\$20,981,688		
	Total	\$51,231,761		Total	\$330,284,214		