

# SUSTAINABLE PRODUCTION OF ETHYLENE OXIDE

PART 3: CHEN 30032

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## Abstract

This study outlines the design and economic-environmental evaluation of a sustainable ethylene oxide (EO) production facility with a target production rate of 150 kt yr<sup>-1</sup>, located in Freeport, Texas. The project began by collating the detailed design of individual process units, ranging from the reactor and absorption sections to EO purification and air separation, into an integrated plant-wide system. A rigorous process optimization was then performed using Bayesian methods, focusing on reducing reactor size and purge stream losses, which led to an annualized cost saving of nearly \$3 million. Following this, a comprehensive plant layout was developed, prioritising operational efficiency, safety, and expandability. Strategic zoning was applied to separate high-risk units like the reactor and cryogenic oxygen plant, while a centralised tank farm and ancillary infrastructure were optimised for logistics and hazard minimization. Subsequently, thermal integration was conducted using pinch analysis, which completely eliminated the need for hot utilities and significantly reduced cold utility consumption, particularly for cryogenic refrigeration, through an advanced heat exchanger network. In terms of economics the plant achieves a yearly revenue of \$207 million against a manufacturing cost of \$175 million, yielding a profit of \$32 million per year and a discounted cash flow rate or return of 15%. These figures underscore the plant's strong commercial viability. Sustainability was central to the design process. A robust investigation into the environmental impact was conducted through a life cycle assessment (LCA), revealing a total carbon footprint of 432,900 tonnes CO<sub>2</sub>-equivalent per annum. This footprint was substantially reduced through intelligent waste management strategies, carbon capture, and minimization of raw material consumption via process integration and recycle strategies. Key initiatives included closed-loop catalyst regeneration, wastewater detoxification, flare gas energy recovery, and inert gas reuse. Process integration was a key aspect in terms of improving economic efficiency and environmental sustainability. The generation of a maximum energy recovery heat exchanger network allowed for the elimination of any hot utility requirements and significantly reduced the cold utility from 208650 to 190273 kW, with a significant reduction in the expensive cryogenic refrigeration to approximately 30% of its original value. In summary, this project presents a modern EO facility design that harmonizes economic performance, process safety, and environmental responsibility, offering a model for sustainable chemical manufacturing in the 21st century.

# 1 Introductory Context and Major Changes

## 1.1 Scope of project

An optimisation and feasibility study will evaluate potential process configurations and operating conditions to maximise EO yield, minimize costs, and enhance operational safety. This involves capital and operating cost estimations, along with a thorough optimisation study to verify the economic viability and safety of the plant operation. Sustainability assessments, such as life-cycle analysis (LCA) and environmental impact evaluations, will also be conducted to minimize the facility's carbon footprint.

Engineering and plant layout will encompass the development of detailed process flow diagrams (PFDs), piping and instrumentation diagrams (P&IDs), and both 2D and 3D site layouts to ensure safe, efficient, and practical plant operation. Major equipment, including reactors, absorbers, compressors, distillation towers, and heat exchangers, will be specified alongside essential support facilities such as storage tanks, utilities, and ancillary buildings. Safety strategies and protocols will follow best practices, involving hazard and operability studies (HAZOP) and clear arrangements for plant commissioning, start-up, and shutdown.

The project will prioritise sustainability and social responsibility by integrating measures to capture and either reuse or sequester carbon dioxide emissions. Waste management strategies will include recycling spent catalysts and implementing comprehensive wastewater treatment solutions. Furthermore, stakeholder engagement plans will be developed to address community and environmental concerns proactively. Occupational health and safety will also be reinforced through rigorous hazard identification processes, robust emergency response protocols, and extensive worker training programs.

Lifecycle and economic evaluations will be conducted, employing profitability assessments based on discounted cash flow analysis, payback periods, and investment rate-of-return calculations. Sensitivity and parametric analyses will be carried out to examine the effects of fluctuations in raw material and utility pricing, thereby capturing the range of potential economic uncertainties.

Overall, the project scope is designed to ensure that the proposed EO production facility in Freeport, Texas, meets contemporary industrial standards, complies fully with rigorous safety regulations, and achieves both economic viability and environmental stewardship.

## 1.2 Reactor section

The major change in the reactor section was a slight decrease in selectivity compared to the Part 1 estimate. The selectivity was reduced from 85% to 83.9%. Also, the use of the inhibitor ethylene dichloride was added into the design. It is assumed that the inhibitor will be added along with the fresh methane feed. The amount of ethylene dichloride is very small, and it is assumed that no amount leaves the reactor, so it is not considered in the stream table.

## 1.3 Absorption Unit

Major modifications made to the ethylene oxide absorption unit design are focused on the solvent recovery column, T-104 where the original distillation column has been replaced with a flash column. In Part 1 of the design, the performance of the absorption process was simply evaluated based on split fraction assumptions without considering actual thermodynamic behaviour. Simulation results derived from an appropriate thermodynamic model in Part 2 confirms the presence of light non-condensable gases in the EO-rich solvent exiting the absorption column which was previously neglected. As a result, using a distillation column would require a substantial condenser duty to condense these gases for EO-water separation as demonstrated by shortcut calculations using the Underwood equation. Further justification for this modification comes from the Fenske equation and Gilliland correlation which predicted an unrealistically low number of separation stages of 2 stages,

indicating that the distillation column was a severe overdesign and economically unfeasible. Initially, concerns were raised about the flash column's ability to achieve high-purity separation compared to distillation. However, simulation results confirmed an almost perfect split between EO and water, enabling the pure water stream to be recycled back into the absorption column.

## 1.4 Carbon Capture Unit

In the detailed design of the columns in part 2, piperazine promoted potassium carbonate was found to be a more suitable solvent than the MEA promoted potassium carbonate used in part 1. This new solvent operated a lean mass flowrate of 146700 kg/hr. Piperazine was selected as it has a greater promoting effect than MEA and is significantly more stable in system. MEA was found to be unsuitable as it reacts irreversibly with oxygen and there is a significant oxygen flow through the absorption column.

Due to the large pressure gain required between the desorption column and the absorption column, as well as the very low NPSH available leaving the desorption column, two pumps were required to raise the pressure back to 21 bar with the second pump being a multistage pump. Optimization of this section found that the reboiler duty greatly decreased when reducing the pressure of the desorption column, and the desorption column thus had its operating pressure reduced to 0.8 bara.

## 1.5 EO Purification Units

The initial downstream purification units consisted of distillation columns T-105 and T-106 to purify and obtain the 99.5 wt% Ethylene Oxide with an annual production target of 150 kt a<sup>-1</sup>. The purpose of T-105 is to remove traces of light gasses present in the feed, with the bottoms consisting of Ethylene Oxide and Water being fed into T-106 which further separates these two species to form the purified Ethylene Oxide stream in the overheads. Due to the negligible amounts of light gasses entering T-105, it was decided to entirely remove column T-105 due to its redundancy and only design T-106, which is a simple distillation column consisting of a partial reboiler and partial condenser. The partial condenser consists of a vapor and liquid distillate streams, whereby the non-condensable light gasses escape through the vapor stream, hence there is no requirement of total condensation. The liquid distillate stream will consist of the final purified Ethylene Oxide product stream. As a column was removed, distillation column T-106 will from this point onwards be renumbered T-105 and cryogenic distillation column T-107 will be renumber T-106.

## 1.6 Air Separation Unit

In Part 2 the preliminary conceptual design of the air separation unit was developed and expanded into a working system to convert atmospheric air into purified oxygen, with a purity of over 99.5%. It was established in the design that a series of pretreatment steps are required for optimal air separation, firstly an initial flash stage (T-107) to remove water from the air and a subsequent adsorption step (T-108) to remove carbon dioxide, both of which would freeze and damage the internals of the cryogenic system. The new unit names follow the convention laid out previously. The cryogenic distillation column (T-106) was designed to deliver 500 kmol hr<sup>-1</sup> of purified oxygen and can accommodate fluctuations in demand.

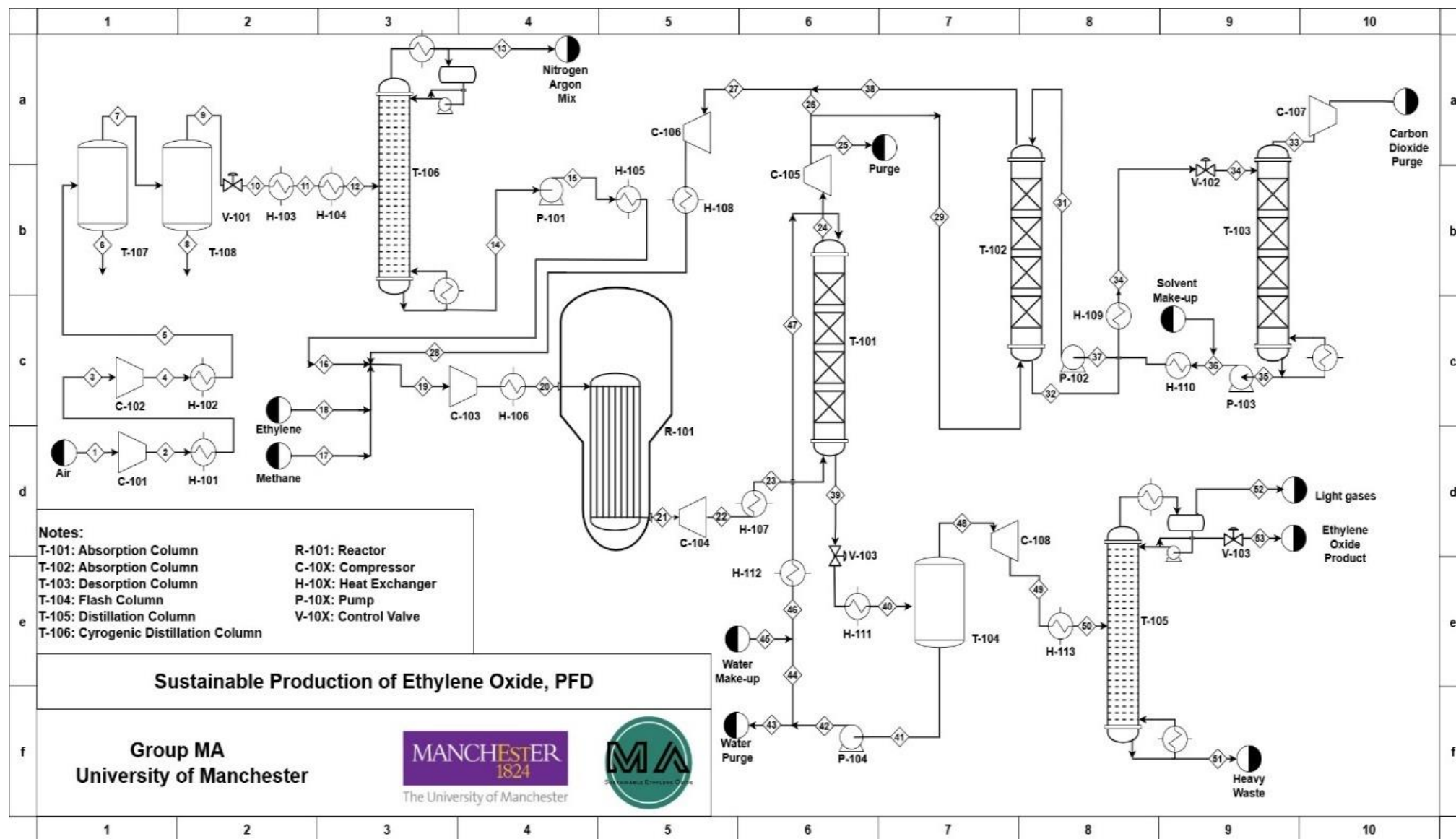


Figure 1.1 – Updated PFD of ethylene oxide process



## 2 Process Optimisation

An economic optimisation was performed on a small sub section of the chemical plant. The main goal of this section was to optimise the values of the most significant variables which affected the cost of the plant.

### 2.1 Section selection

In order to select the most suitable section to optimise, first a breakdown analysis of the operating and capital cost was required. Yoon et al (2024) breakdown the capital cost of a conventional ethylene oxide plant and present the percentage share of the total capital investment (TCI) by process unit.

Figure 2.1 shows that largest portion of capital investment goes towards the heat exchanger at 38.4%. This highlights the importance of optimising the design of heat exchangers. However, in this report the optimisation of a small subsection of the plant is required and the heat exchangers are found throughout the entire process. Therefore, this section will not look at the optimisation of the heat exchanger sizing.

The second highest share of the capital cost is the reactor at 24.7%. This is a significant proportion of the total cost; it was therefore decided that the reactor size would be an important variable to consider in order to minimise the capital cost of the plant.

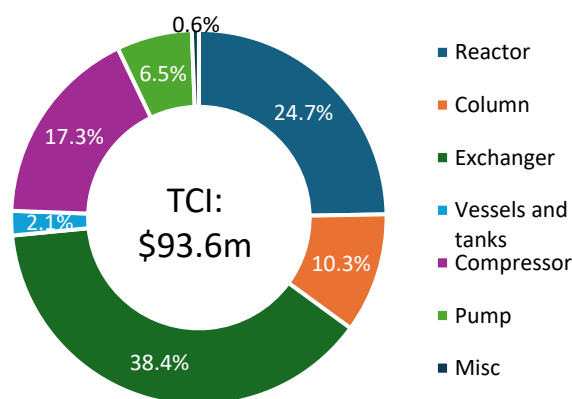


Figure 2.1 – Total capital investment of an ethylene oxide plant by process equipment (Yoon et al., 2024)

Yoon et al (2024) also provide a breakdown of the operating cost of the conventional ethylene oxide plant. Figure 2.2 shows the annualised operating cost (AOC) breakdown by material and utility. It is clear that the cost of ethylene dominates the operating costs of the plant. Hence it was decided that the fresh feed flowrate and the purge fraction were also important variables to optimise as they were key variables that could reduce the requirement of ethylene. The conversion and selectivity of the reactor also significantly affect the ethylene requirement, which further justified the importance of reactor optimisation. An annual operating cost of \$99.1m was calculated using the target of 163 kt per year of EO and cost of \$608 per tonne of EO produced

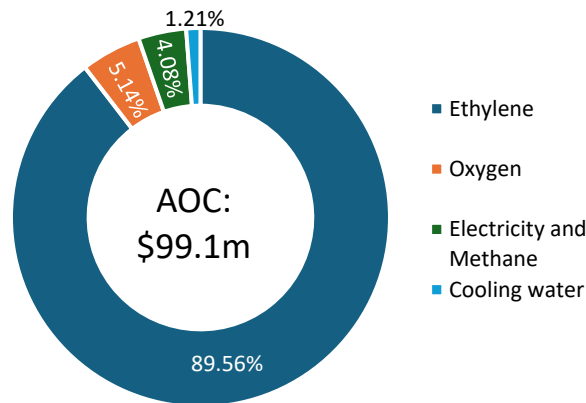


Figure 2.2 – Annualised operating cost (AOC) of an ethylene oxide plant by raw material and utility (Yoon et al., 2024)

Although it was decided that the optimisation of the reactor section was to be completed first, it is still imperative that the rest of the process is optimised as there are many more opportunities to reduce cost. The optimisation of the reactor was just deemed the most important based on the information provided.

Figure 2.3 illustrates a simplified diagram of the process with the selected optimisation variables highlighted in red. A Python model of the reactor and recycle loop was created utilising the detailed reactor model from Part 2 and assuming split fractions for the absorber and carbon capture sections. Further information of the simulation model is detailed in Section 2.5.1 and the justification of the variable selection is entailed in Section 2.2.

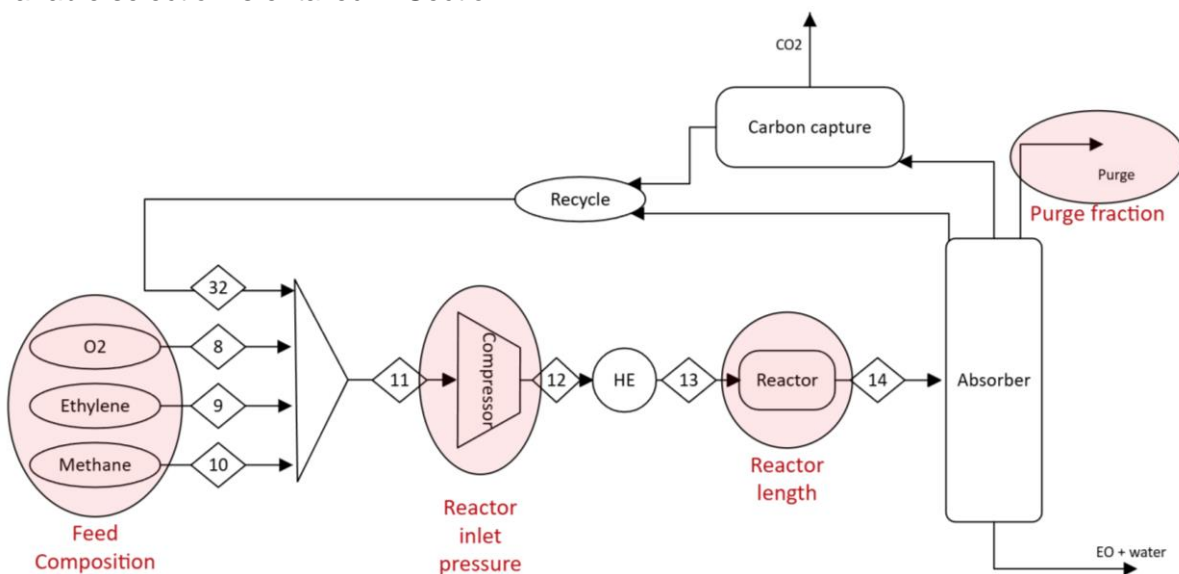


Figure 2.3 – Simplified diagram of the subsection of the plant optimised. Optimisation variables highlight in red.

## 2.2 Optimisation variables

The optimisation problem defines the variables as 6 distinct variables. These are the reactor length, the inlet pressure, the purge fraction and the fresh feed flow rate of ethylene, oxygen, and methane. Based on the sensitivity analysis from the Part 2 Reactor design, it was seen that increasing the reactor length also increases the conversion whilst decreasing the selectivity after a certain length. The optimal length varies depending on the reactor feed composition and the cost of increasing reactor volume. Therefore, it was determined that the reactor length was a suitable variable to optimise.

The inlet pressure of the reactor was a key variable that influenced the kinetics of all reactions. The Part 2 sensitivity analysis showed that a high pressure increased conversion but also decreased



selectivity. An inlet pressure that is too low could also be problematic as the pressure drop within the reactor could become problematic. Therefore, the inlet pressure was determined to be an important optimisation variable. The coolant temperature could also have been used for the same reason, however for safety and catalyst preservation reasons the coolant temperature was fixed at a low temperature.

The purge fraction and the ethylene feed flowrate can both be adjusted to minimise ethylene loss based on material balance fundamentals. The oxygen flowrate was important to control as adjusting the ethylene input will change the ratio of feed entering the reactor. The oxygen concentration was also a key variable in the reaction kinetics. The cost of oxygen also made up the second largest share of the operating costs of the plant.

The flowrate of methane was also chosen as an optimisation variable as the purge fraction would change the requirement of methane into the system. Methane is also important to ensure that the flammability limit within the reactor was not exceeded.

The aforementioned variables are tabulated in Table 2.1 with their respective bounds and units. The table also includes a summary of their significance

Table 2.1 – Summary table of optimisation variables

Variable	Symbol	Bounds	Units	Significance
Fresh C <sub>2</sub> H <sub>4</sub>	$F_{C_2H_4}$	140-190	mol s <sup>-1</sup>	EO yield & feedstock cost
Fresh O <sub>2</sub>	$F_{O_2}$	130-170	mol s <sup>-1</sup>	EO yield & feedstock cost
Fresh CH <sub>4</sub>	$F_{CH_4}$	30-100	mol s <sup>-1</sup>	Maintains safe O <sub>2</sub> concentration
Reactor Length	$L_R$	8-16	m	Conversion/selectivity, catalyst requirement and capital cost
Reactor Inlet P	$P_{in}$	15-21	atm	Influences conversion/selectivity & pressure drop
Purge Fraction	$\phi$	0.006-0.05	–	Affects inert build up & feed stock cost

## 2.3 Objective function

The purpose of this optimisation was to minimise the operating and capital cost whilst maintaining safe operating conditions and meeting production targets. Hence, an objective function that reflected this purpose was created. The annualised capital cost of the reactor was summed with annual operating cost of the plant to give the partial annualised cost (PAC) of the section, shown in Equation 2.1. The Equation also includes penalty terms to ensure safe operation and sufficient EO production. Utilities were not considered in the objective function due to their small share in the operating cost.

$$PAC = CRF \times C_{cap} + C_{rm} + C_{cat} + \sum \mathcal{P}_j \quad \text{Equation 2.1}$$

where:

- CRF is the capital-recovery factor over the plant lifetime  $N$  at discount rate  $i$

$$CRF = \frac{i(1+i)^N}{(1+i)^N - 1}$$

- $C_{cap}$  is the installed capital cost of the reactor.
- $C_{rm}$  is the annual raw-material cost (ethylene, oxygen, methane).
- $C_{cat}$  is the annualised catalyst make-up and initial cost (silver/Al<sub>2</sub>O<sub>3</sub>).
- $\mathcal{P}_j$  is the penalty function for the constraint  $j$

### 2.3.1 Operating cost

The operating cost per annum only used the raw material costs as the change to the utilities cost would be negligible in comparison to the change in raw material. The calculation is shown in Equation 2.2.

$$C_{\text{rm}} = \sum_{j \in \{\text{C}_2\text{H}_4, \text{O}_2, \text{CH}_4\}} (\dot{m}_j \times p_j) \times 8000 \text{ h/yr} \quad \text{Equation 2.2}$$

where  $\dot{m}_j$  (kg/h) is the steady-state mass flow of species  $j$  into the system and  $p_j$  its unit price (\$/kg). A fixed cost of oxygen based on market price was used instead of assuming the cost of oxygen production.

In this equation, the cost of oxygen is assumed to be the purchased cost of oxygen in order to simplify the simulation model. The price of raw material is the same as the market research values from Part 1 of the report. These are \$0.69/kg, \$0.1/kg and \$0.15/kg for ethylene, oxygen and methane respectively.

### 2.3.2 Capital cost

The annualised capital cost of catalyst make up is given in Equation 2.3.

$$C_{\text{cat}} = \frac{(1 - r_{\text{rec}}) m_{\text{Ag}} p_{\text{Ag}} + p_a m_{\text{cat}}}{L_{\text{cat}}} \quad \text{Equation 2.3}$$

Where the catalyst recovery  $r_{\text{rec}} = 0.95$ , the price of silver is  $p_{\text{Ag}} = \$1\,060/\text{kg}$ , the total support and catalyst manufacture price is  $p_{\text{mfg}} = \$15/\text{kg cat}$ . The mass of silver,  $m_{\text{Ag}}$ , is computed from bed volume, bulk density ( $1\,260 \text{ kg m}^{-3}$ ), void fraction (0.45) and 25 wt % Ag.

The capital cost of the reactor was calculated using the correlation provided by Turton (2002). The correlation approximates the price of a reactor based on the area of the reactor. The price is then multiplied by the CEPCI ratio to determine the current cost of the reactor. The most recent publicly available CEPCI in 2024 was 798.6 and in the year 2002 a CEPCI value of 395.6 is used, giving an inflation factor of 2.019

$$C_{\text{cap}} = 4.57 \times 10^4 \times A_R^{0.67} \times 2.019 \quad \text{Equation 2.4}$$

### 2.3.3 Penalty and inequality constraints

Penalties ensure solutions remain feasible yet keep the search space continuous for optimisation. In this study, a quadratic penalty term was used to penalise boundary violations, shown in Equation 2.2.

$$\mathcal{P}_j = \begin{cases} 0, & c_{j,\min} < c_j < c_{j,\max} \\ \alpha_j (c_{j,\min} - c_j)^2, & c_j < c_{j,\min} \\ \alpha_j (c_j - c_{j,\max})^2, & c_j > c_{j,\max} \end{cases} \quad \text{Equation 2.2}$$

Where:

- $c_j$  is the value of the constrained variable for constraint  $j = 1, \dots, 5$
- $\mathcal{P}_j$  is the penalty function for the constraint  $j$
- $c_{j,\min}$  and  $c_{j,\max}$  are the lower and upper boundary value for the constraint  $c_j$  respectively
- $\alpha_j$  is the penalty scale of the constraint  $j$

Table 2.2 – Inequality constraints used in penalty function

$j$	Constraint	Admissible range $[c_{\min}, c_{\max}]$	Engineering basis	Penalty scale $\alpha_j$
1	O <sub>2</sub> mole fraction at reactor inlet	0.05 – 0.09	Lower bound avoids O <sub>2</sub> starvation & hot spots; upper bound below flammability limit for C <sub>2</sub> H <sub>4</sub> /O <sub>2</sub> /CH <sub>4</sub> mixtures. (Ulmann, 2012)	$1 \times 10^{10}$
2	C <sub>2</sub> H <sub>4</sub> mole fraction in reactor inlet	0.15 – 0.40	The safe range of operation given by Ulmann (2012)	$1 \times 10^9$
3	EO production rate	150-170 kt yr <sup>-1</sup>	Matches production target and downstream purification capacity.	$1 \times 10^7$
4	Reactor tube skin temperature	$\leq 523$ K	Ensure a long catalyst life and reduce the chance of hotspot and runaway reactions (Nawaz, 2016)	$1 \times 10^7$
5	Reactor conversion	7% – 15%	Ulmann (2012) recommend maintaining the reactor conversion within the given range to ensure safe operation and high yield.	$1 \times 10^7$

## 2.4 Optimisation methodology

### 2.4.1 Simulation model

The simulation model of the plant subsection was made in Python using a sequential modular approach. The reactor code from Part 2 was reused in the model. The reactor effluent enters the absorber which splits it into a rich solvent stream that contained mainly EO/water and a lean gas stream that contained the remaining gas and some water from the stream. The streams were split based on the split fraction of the absorber Part 1 design as the Part 2 design lost too much ethylene making the process economically infeasible. The lean gas stream is split into three streams, a purge stream, a carbon capture stream and direct recycle stream. The carbon capture stream has a fixed amount of CO<sub>2</sub> and other species removed based on the Part 2 design for the carbon capture section. The rest of the stream is combined with the recycle to be fed back into the reactor along with the fresh feed.

As the model contains a recycle stream, the recycle stream needs to first be converted into a tear stream. Then the species flow rates between the streams needs to converge to a single value. An initial value for the tear stream entering the reactor was assigned based on the material balance from Part 1. The Anderson mixing acceleration algorithm provided by the SciPy library was used to close the loop.

### 2.4.2 Optimisation algorithm

With the flowsheet successfully able to simulate the sub section of the plant the next step was to solve the optimisation problem. As a sequential modular approach was taken to make the simulation model, a derivative free optimisation algorithm was required. Initially, differential evolution and simulated annealing were trialled. However, using these methods would have taken a very long time to converge to a value.

Bayesian optimisation, implemented through the Optuna Python library, overcomes these shortcomings. The method treats the flowsheet as a black box and, after each evaluation, updates a probabilistic surrogate that predicts the distribution of feasible and economically attractive regions. An acquisition function proposes the next experiment by weighing the chance of reducing

cost against the uncertainty of the surrogate. Thus, the search initially explores widely, learning the penalty cliffs associated with flammability and throughput, and later narrows its focus to the most promising regions.

## 2.5 Optimisation result and discussion

The final optimisation results can be found in Table 2.3. A saving of almost \$3 million per year can be seen from the annualised cost based on the changes made from the optimisation.

Table 2.3 – Final optimisation results and optimised variable values compared with original values.

Variable	Original value	Optimised value
Objective Function (PAC)	\$121,007,000 per year	\$117,714,000 per year
Purge fraction	0.009	0.0107
Reactor length	12 m	14.4 m
Reactor inlet pressure	21 bara	18.5 bara
Fresh C <sub>2</sub> H <sub>4</sub>	176.7 mol s <sup>-1</sup>	168.9 mol s <sup>-1</sup>
Fresh O <sub>2</sub>	158.9 mol s <sup>-1</sup>	157.0 mol s <sup>-1</sup>
Fresh CH <sub>4</sub>	55.6 mol s <sup>-1</sup>	47.1 mol s <sup>-1</sup>

Figure 2.4 illustrates the decrease in the objective value as the number of optimisation trials increased. It is clear that optimisation searches the multi-dimensional space with a high variability in the value of the variables. This causes the objective values to seem extremely high as the space that the optimisation algorithm was searching in was within the penalty region. As the number of trials increases the optimisation algorithm finds a local optimal value, but at the same time it tries to explore outside the region hence the high objective function values. The optimisation trial was stopped at 547 trials as the optimisation had found the local optimal value and was no longer exploring outside the region.

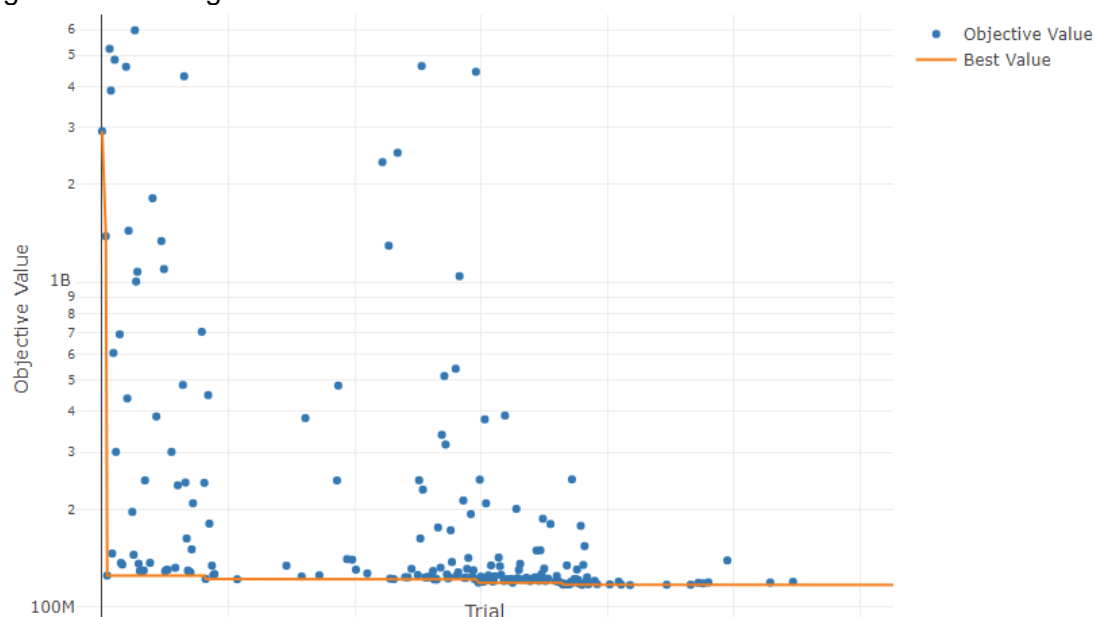


Figure 2.4 – Plot of objective value by trial number in optimisation study. The orange line shows the objective value of best parameter combination as the number of trial increases.

The Optuna library also allows the user to understand the importance of each variable or hyperparameter in the optimisation study. This is based on the variance of the objective function with a change in the given variable/hyperparameter. In Figure 2.5, it can be seen that the flow rate of the reactants are the top two most important variables in the study. A further investigation into the two most important variables can be done by plotting the contour plot of the surrogate objective function approximation with the reactant feed flowrates. This is illustrated in Figure 2.6. It is clear from the figure that penalty boundaries arise when the composition of the feed escapes the region between

150 – 165 mol s<sup>-1</sup> for the oxygen feed flowrate and above 160 mol s<sup>-1</sup> for the ethylene feed. This can be explained as values too low or too high will either cause the plant production capacity to not be met or the flammability limit in the reactor to be exceeded.

Hyperparameter Importance

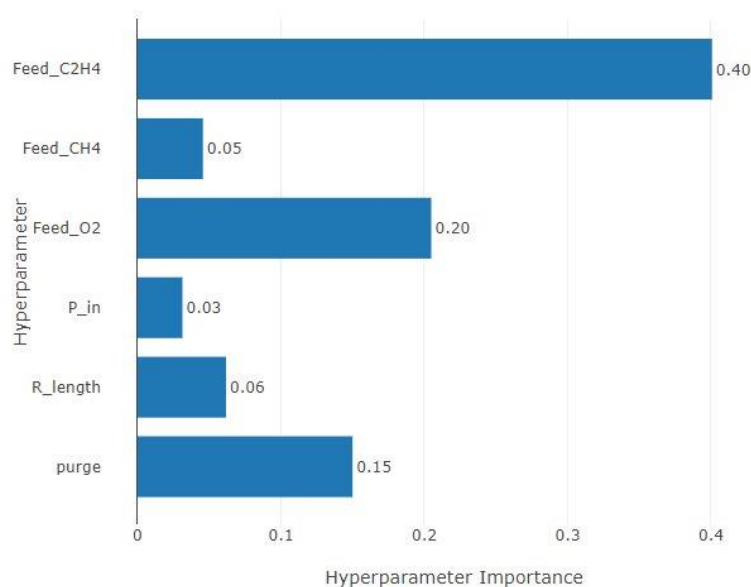


Figure 2.5 – Bar chart comparing the importance of each variable/hyperparameter in the optimisation study.

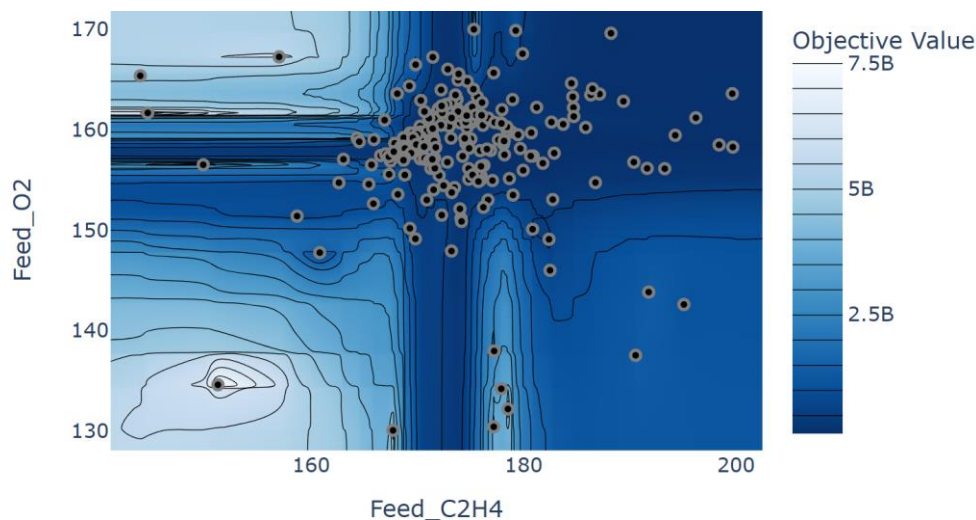


Figure 2.6 – Contour plot of the surrogate model's objective value approximation (\$ yr<sup>-1</sup>) with the fresh feed flowrate of oxygen and ethylene (mol s<sup>-1</sup>). The black dots represent the optimisation trial values explored.

Based on Figure 2.5 and the final optimisation variable values it is clear that the optimisation study found that the operating costs were more important to optimise compared to the capital cost. However, this could be due to the assumptions and simplifications made in determining the objective function as the only capital cost considered was that of the reactor. If the other units such as the absorber, heat exchanger network and carbon capture units, were modelled in more detail may have more considerable affect in deciding the optimal value.

In conclusion, a simple optimisation study was performed on reactor-separation-recycle loop and a \$3 million per saving was found. While a saving was found, it is extremely likely a further saving could be found if a more rigorous optimisation approach was used, such as modelling the system in an equation orientated approach rather than using a sequential modular one as this would not limit the optimisation to use of black box optimisation algorithms. An optimisation on the downstream sections would be recommended next to further reduce the cost of the process.

### 3 Mass and Energy Balance Table

Stream	1	2	3	4	5	6	7	8	9	10	11	12	13	
Vapour Quality	1.0	1.0	1.0	1.0	1.0	0.0	1.0	0.0	1.0	1.0	1.0	0.0	0.0	
Temperature (C)	27.8	143.9	50.0	179.5	35.0	25.0	25.0	25.0	25.0	-5.8	26.0	-183.3	-189.5	
Pressure (bar)	1.0	2.6	2.6	6.7	6.7	5.0	5.0	5.0	5.0	3.0	3.0	3.0	2.0	
Total Molar Flow (kmol/hr)	2809.4	2809.4	2809.4	2809.4	2809.4	84.1	2725.3	0.2	2725.1	2725.1	2725.1	2725.1	1897.7	
Total Mass Flow (kg/hr)	80436.0	80436.0	80436.0	80436.0	80436.0	1514.7	78921.3	4.3	78917.0	78917.0	78917.0	78917.0	53161.3	
Total Heat Flow (MW)	-5.6	-2.9	-5.1	-2.1	-6.2	-6.7	0.0	0.0	0.0	-0.7	0.0	-8.7	-6.1	
Species Molar Flow (kmol/hr)														
ETHYLENE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
EO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
METHANE	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
WATER	84.3	84.3	84.3	84.3	84.3	84.1	0.2	0.2	0.0	0.0	0.0	0.0	0.0	
EG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
ARGON	25.3	25.3	25.3	25.3	25.3	0.0	25.3	0.0	25.3	25.3	25.3	25.3	0.0	
Solvent mixture - CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
OXYGEN	571.1	571.1	571.1	571.1	571.1	0.0	571.1	0.0	571.1	571.1	571.1	571.1	0.0	
NITROGEN	2128.7	2128.7	2128.7	2128.7	2128.7	0.0	2128.7	0.0	2128.7	2128.7	2128.7	2128.7	1897.7	
Stream	14	15	16	17	18	19	20	21	22	23	24	25	26	27
Vapour Quality	0.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Temperature (C)	-176.8	-176.0	50.0	50.0	50.0	48.9	210.0	210.0	269.0	68.5	63.4	63.4	63.4	63.4
Pressure (bar)	3.0	18.5	18.5	18.5	18.5	18.5	18.5	12.5	21.5	21.5	21.0	21.0	21.0	21.0
Total Molar Flow (kmol/hr)	827.4	827.4	827.4	169.6	608.0	18835.3	18835.3	18617.1	18617.1	18617.1	17550.1	158.0	14759.6	17230.3
Total Mass Flow (kg/hr)	25755.6	25755.6	25755.6	2720.2	17057.8	468890.9	468890.9	468890.9	468890.9	468890.8	434223.5	3908.0	365181.9	423357.2
Total Heat Flow (MW)	-2.7	-2.7	0.2	-3.5	9.1	-367.8	-330.8	-380.1	-365.3	-414.0	-390.4	-3.5	-328.3	24.6
Species Molar Flow (kmol/hr)														
ETHYLENE	0.0	0.0	0.0	0.0	608.0	4463.0	4463.0	3927.5	3927.5	3927.5	3894.6	35.1	3275.3	3855.0
EO	0.0	0.0	0.0	0.0	0.0	6.9	6.9	443.4	443.4	443.4	7.0	0.1	5.9	6.9
METHANE	0.0	0.0	0.0	169.6	0.0	8853.0	8853.0	8853.0	8853.0	8853.0	8764.9	78.9	7371.3	8683.5
CO2	0.0	0.0	0.0	0.0	0.0	2157.4	2157.4	2355.7	2355.7	2355.7	2332.4	21.0	1961.6	2157.4
WATER	0.0	0.0	0.0	0.0	0.0	247.7	247.7	446.0	446.0	446.0	250.8	2.3	210.9	247.7
EG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	25.3	25.3	25.3	0.0	0.0	432.5	432.5	432.5	432.5	432.5	410.9	3.7	345.6	407.2
Solvent mixture - CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OXYGEN	571.1	571.1	571.1	0.0	0.0	2443.6	2443.6	1928.0	1928.0	1928.0	1889.5	17.0	1589.1	1872.5
NITROGEN	231.0	231.0	231.0	0.0	0.0	231.0	231.0	231.0	231.0	231.0	0.0	0.0	0.0	0.0



Stream	28	29	30	31	32	33	34	35	36	37	38	39	40
Vapour Quality	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0
Temperature (C)	50.0	65.0	65.0	65.0	32.1	40.0	31.2	87.4	87.5	62.6	65.0	63.4	96.5
Pressure (bar)	21.0	21.0	21.0	21.0	21.0	1.0	1.0	1.0	3.0	3.0	21.0	21.0	21.0
Total Molar Flow (kmol/hr)	17230.3	2632.5	5609.9	5618.9	5618.9	161.8	5618.9	5616.8	5616.8	5625.5	2470.7	61077.2	61077.2
Total Mass Flow (kg/hr)	423357.2	65133.5	146653.7	153610.1	153610.1	6958.3	153610.1	146835.9	146835.9	147085.3	58175.3	1116271.2	1116271.2
Total Heat Flow (MW)	24.6	-92.1	-4.4	-413.0	-73.7	-16.8	-56.9	-470.0	-470.0	0.0	-74.4	-4742.2	-4697.6
Species Molar Flow (kmol/hr)													
ETHYLENE	3855.0	584.2	4.7	6.6	6.6	4.5	6.6	11.7	11.7	18.9	579.7	33.4	33.4
EO	6.9	1.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.1	455.0	455.0
METHANE	8683.5	1314.7	1.1	3.5	3.5	2.5	3.5	1.1	1.1	1.8	1312.2	88.5	88.5
C02	2157.4	349.9	0.1	2.3	2.3	154.0	2.3	0.2	0.2	0.1	195.9	23.6	23.6
WATER	247.7	37.6	4475.8	4324.4	4324.4	0.8	4324.4	4475.8	4475.8	4475.8	36.8	60185.1	60185.1
EG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	407.2	61.6	0.6	2.5	2.5	0.0	2.5	0.6	0.6	1.5	61.6	21.6	21.6
Solvent mixture - C02	0.0	0.0	1127.6	1279.6	1279.6	0.0	1279.6	1127.4	1127.4	1127.4	0.0	0.0	0.0
OXYGEN	1872.5	283.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	283.4	38.6	38.6
NITROGEN	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	231.4	231.4
Stream	41	42	43	44	45	46	47	48	49	50	51	52	53
Vapour Quality	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0	0.1	0.0	1.0	0.0
Temperature (C)	96.5	97.2	97.2	97.2	60.3	75.3	60.3	96.5	272.6	39.0	39.0	39.0	39.0
Pressure (bar)	1.0	21.0	21.0	21.0	21.0	21.0	21.0	1.0	4.1	4.1	4.1	4.1	4.1
Total Molar Flow (kmol/hr)	53247.7	53247.7	29273.5	23974.2	36036.0	60010.2	60010.2	7829.5	7829.5	7829.5	7398.5	24.1	406.8
Total Mass Flow (kg/hr)	960390.8	960390.8	527985.6	432405.2	649198.6	1081603.8	1081603.8	155880.4	155880.4	155880.4	137317.3	668.4	17894.7
Total Heat Flow (MW)	-4142.7	-4141.9	-2277.1	-1864.8	-2834.2	-4699.0	-4718.5	-473.5	-459.5	-564.0	-555.2	-0.9	-8.6
Species Molar Flow (kmol/hr)													
ETHYLENE	1.0	1.0	0.6	0.5	0.0	0.5	0.5	32.4	32.4	32.4	23.3	8.6	0.5
EO	41.4	41.4	22.8	18.6	0.0	18.6	18.6	413.6	413.6	413.6	8.3	0.0	405.3
METHANE	0.8	0.8	0.4	0.4	0.0	0.4	0.4	87.7	87.7	87.7	80.9	6.5	0.3
C02	0.6	0.6	0.3	0.3	0.0	0.3	0.3	22.9	22.9	22.9	16.5	6.1	0.3
WATER	53202.6	53202.6	29248.7	23953.9	36036.0	59989.9	59989.9	6982.5	6982.5	6982.5	6979.3	2.9	0.3
EG	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ARGON	0.1	0.1	0.1	0.0	0.0	0.0	0.0	21.5	21.5	21.5	21.5	0.0	0.0
Solvent mixture - C02	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
OXYGEN	0.2	0.2	0.1	0.1	0.0	0.1	0.1	38.4	38.4	38.4	38.4	0.0	0.0
NITROGEN	1.0	1.0	0.5	0.4	0.0	0.4	0.4	230.5	230.5	230.5	230.5	0.0	0.0

## 4 Process/Energy Integration

### 4.1 Introductory context and methodology outline

In the chemical industry the economics and sustainability of a process are often dictated primarily by the energy and utility requirements of the plant. In 2018 it was found that the industrial sector was responsible for 55% of world energy consumption and the largest proportion of that (12%) was due to the chemical industry (Hydrocarbon Engineering (2019)). It is for this reason that strategies must be put in place to reduce energy consumption, with the objective of improving industrial efficiency and sustainability. By reducing energy consumption, the plant can lower both operating costs and environmental impacts, whilst reducing the reliance on external supply chains for fossil fuel production which fluctuate frequently (Global monthly fossil fuel price index by fuel (2023)) providing an edge in the market in terms of sustainability and economic return.

Process integration plays the key role in achieving these objectives, as it enables maximum internal heat recovery and minimizes the need for external utilities through the systematic optimisation of heat and material flows. This section will identify minimum utility requirements based on a selected minimum temperature difference for heat transfer, subsequently using these targets as a guidance for optimisation of the overall heat exchanger network aiming to reduce reliance on utilities and minimise operating and capital cost of the network. This will be carried out using the software package SPRINT, which allows for the identification of utility targets and development of an optimal maximum energy recovery heat exchanger network (MER HEN).

### 4.2 Identification of integration areas

To facilitate the energy integration of the process, first the system must be analysed and streams requiring either heating or cooling must be identified. This was carried out using the plant simulation software ASPEN. The streams used for integration are listed in Table 4.1, showing the heat requirements and temperature the occur at.

When extracting streams, to allow for simulation and optimisation of the problem some assumptions must be made, they are summarised below:

- Assume constant mass flow/density and specific heat capacity of streams independent of temperature change.
- Assume isothermal heat changes such as those experienced in condensers and reboilers or in the isothermal reactor, experience a small temperature change of 1 °C.
- It is assumed that the operation is in steady state and there is a linear relationship between enthalpy and temperature change, with no heat loss to the environment.
- To facilitate the design of the system it is assumed that utilities are available and occur at necessary flowrates and temperatures.

Table 4.1: Streams Extracted for Integration

Stream number	Name	Stream Type	Supply Temperature (°C)	Target Temperature (°C)	Stream Duty (kW)	Heat Capacity flow/CP (kW °C <sup>-1</sup> )
1	initial air cool - post compression	Hot	143.9	50.0	2154.8	22.9
2	second air cool - post compression	Hot	179.5	35.0	4064.5	28.1
3	R-101 effluent cooling	Hot	210.0	68.5	33807.4	238.9
4	R-101 coolant	Hot	211.0	210.0	36400.0	36400.0
5	recycle loop cooling	Hot	63.4	50.0	3470.3	258.5
6	T-101 solvent cooling	Hot	75.3	60.3	19480.3	1299.5
7	T-105 feed cooling	Hot	272.6	39.0	104569.0	447.6
8	T-103 feed cooling	Hot	65.0	31.2	3362.6	99.5
9	T-102 solvent cooling	Hot	87.5	62.6	2452.8	98.5

10	T-105 condenser	Hot	45.4	44.4	7185.9	7185.9
11	T-106 pre-cool	Hot	-5.8	-183.3	8008.0	45.1
12	T-106 condenser	Hot	-189.3	-190.3	4000.0	4000.0
13	R-101 pre-heat	Cold	49.6	210.0	36919.5	230.2
14	T-104 feed heating	Cold	63.4	96.5	44589.9	1348.1
15	T-105 reboiler	Cold	154.9	155.9	9262.4	9262.4
16	T-103 reboiler	Cold	93.0	94.0	21225.1	21225.1
17	Oxygen feed heating	Cold	-175.8	50.0	2879.1	12.7
18	T-106 reboiler	Cold	-171.0	-170.0	4790.0	4790.0

### 4.3 Minimum approach temperature and Utility requirements

The minimum approach temperature ( $\Delta T_{min}$ ) is a key parameter in the integration problem, this dictates the balance between utility requirement and heat exchange area. (Smith, 2016) SPRINT was used to identify an optimal  $\Delta T_{min}$  with the objective of maximising heat recovery in the process with constraints applied such as minimum cold utility temperature and heat exchange area. The results of this analysis are shown in *Figure 4.1*.

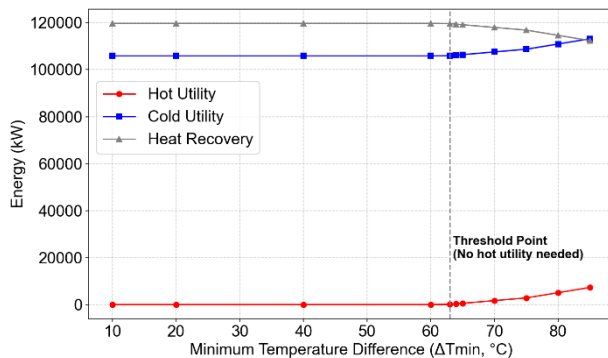


Figure 4.1: Heat requirements based on minimum approach temperature

The analysis conducted with SPRINT, shown in *Figure 4.1*, show that as 63 °C is exceeded, heat recovery reduces and overall utility requirement is increased, particularly hot utility which increases from 0 kW at this point. This shows that this integration problem is not a pinch problem with both hot and cold utility but a threshold problem with only cold utility requirement below a  $\Delta T_{min}$  of approximately 63 °C.

Below the  $\Delta T_{min}$  of 63 °C, marks the point beyond which the process becomes self-sufficient in terms of additional heat supply. Operating under this condition offers several benefits,

including reduced operating costs, lower utility expenditures, and a decrease in initial capital investment due to minimized heat exchanger and utility infrastructure requirements.

The range of  $\Delta T_{min}$  values that defines this threshold problem directly influences both the total heat exchanger area and the required utility temperatures. Specifically, the total heat exchange area is inversely proportional to the chosen  $\Delta T_{min}$ ; a larger temperature difference permits a smaller exchanger area, reducing capital costs. However, increasing  $\Delta T_{min}$  also necessitates colder cold utilities to maintain the required temperature driving force, which may increase operational complexity or cost.

As a result, a careful trade-off must be made between these two opposing factors. The selected  $\Delta T_{min}$  must ensure that cooling water available at the project site, Freeport, Texas, can be used effectively, without requiring auxiliary or lower-temperature utilities. The value of minimum temperature difference will be further discussed once adequate utilities are selected.

### 4.4 Utility Requirement

With the establishment of a threshold problem only cold utilities are required for this process. Due to cryogenic air separation process, very low temperature refrigerants are needed to facilitate the process (in Part 2 nitrogen was selected). In addition to this expensive utility cooling water is used

to provide the cold utility in less extreme circumstances. The temperature of the cooling water is dictated by the environmental conditions.

#### 4.4.1 Cooling water

The temperature of the cooling water is determined based on the climate data for Freeport, Texas, this was gathered using the resource Weather Atlas: Yearly & Monthly Weather - Freeport, TX (2024). The average summer dry-bulb temperature is approximately 27.8°C, with a relative humidity (RH) of around 80%. Using a psychrometric approach and validated through a wet bulb calculator, this results in a wet-bulb temperature of approximately 25°C during peak summer months.

For practical cooling water system design, it is assumed that the cooling water temperature is 3°C above the ambient wet-bulb temperature, which aligns with typical cooling tower performance (Smith (2016)). In this case, the minimum cooling water supply temperature is approximately 28°C, with a typical temperature rise of 10°C, giving a usable cooling water temperature band between 28°C and 38°C.

#### 4.4.2 Refrigeration

Following on from the work conducted in Part 2, due to the very low cryogenic temperatures required for the air separation process only nitrogen is a suitable refrigerant for this process, and this has a minimum safe operation point of approximately -196.15 °C (Smith (2016)).

#### 4.4.3 Utility and $\Delta T_{min}$ summary

Based on the constraints laid out a minimum temperature difference was selected to ensure that the necessary refrigeration could be used at its required temperature range. The  $\Delta T_{min}$  was determined to be 5 °C. This allows for the usage of the necessary utilities and still imposes a constraint on how large the total exchanger area will result in. The final utilities required are tabulated in Table 4.2.

Table 4.2: Utility Temperature summary

Utility	Supply Temperature (°C)	Return Temperature (°C)
Cooling water	28	38
Nitrogen Refrigerant	-196	-195

### 4.5 Utility Targets:

Using SPRINT, the utility targets were established for the process. With the selection of the minimum approach temperature, a balanced Grand composite curve (bGCC) could be plotted to show the optimal distribution of utilities at their required temperature ranges, favouring the lower cost cooling water compared to the other colder utilities. This is presented in Figure 4.2.

The balanced grand composite curve, Figure 4.2, shows an overall minimum cold utility of 109300 KW, which is predominately made up of cooling water. The energy targets for each utility are summarised in Table 4.3. This method of determining utility requirements is more beneficial than simply conducting a more simplistic composite curve as the utilities can be mapped on to a given temperature interval giving a better insight into their distribution. (Smith, 2016).

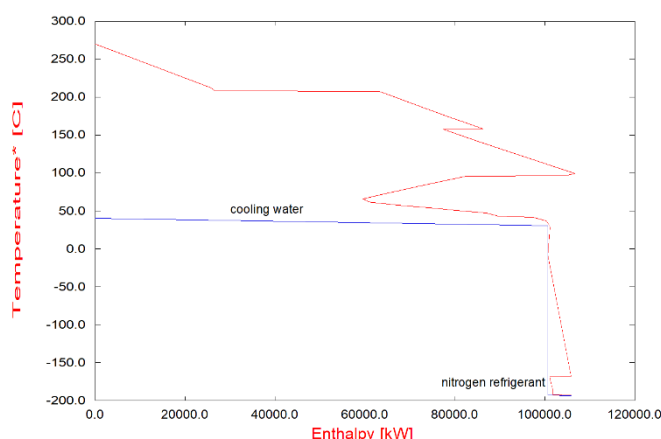


Figure 4.2: Balances Composite curve (red line - process heat, blue line – utility distribution)

Table 4.3: Utility Targets:

Utilities	Target (kW)	
Cooling water	1004176	95.3%
Nitrogen Refrigerant	5114	4.7%
<b>Total</b>	109290 kW	

## 4.6 Heat exchanger Network.

With energy targets and utility distributions established, the construction of a heat exchanger network could begin. The process of generating the network begins with an initial estimation from SPRINT. This initial network gives a starting point for later optimisation which achieves close to maximum heat recovery; however, this network contained many small heat exchangers with areas below and around  $1 \text{ m}^2$  and inefficient utility distribution. To facilitate the optimisation of the MER HEN, arbitrary cost values for each utility were selected to weight the objective function in favour of the much cheaper cooling water, selecting a value  $0.005 \text{ \$ kWh}^{-1}$  and  $10 \text{ \$ kWh}^{-1}$  for cooling water and refrigeration respectively.

To begin and guide the optimisation process all unnecessary heat exchangers were removed to reduce system complexity and unnecessary capital expenditure. Based on the costing correlation presented by Sinnott and Towler (2012), independent of area, an initial charge of \$24,000 would be incurred, so it was economically infeasible to keep small heat exchangers. Along with the removal of unnecessary heat exchangers, unnecessary stream splits were also avoided, so as to reduce the pumping and piping requirements of the MER HEN. The optimisation was carried out by shifting heat loads across utility paths and heat exchanger loops first to maximise heat recovery then to minimise overall cost, where overall cost is a function of both heat exchange area and energy recovery.

The final heat exchanger network resulted in a total cold utility requirement of 190273 kW, which is less than the original target value which implies the system has improved heat recovery compared to the initial estimation. This value is optimal in terms of reducing heat exchange area and utility usage, balancing initial capital costs and operating costs. The number of heat exchanger was reduced from 31 in the initial step, over the course of optimisation to 25, reducing the area requirement and cost of the process.

The MER HEN constructed provides significant improvements on the pre integrated systems in terms of utility usage. Before heat recovery 110239.9 kW of hot utility is required which, due to the threshold nature of the problem, is reduced to 0 kW. Additionally, the overall cooling utility is decreased from approximately 208650 kW down to the previously sated 190273 kW, even though this decrease is not as substantive as the hot utility recovery, it still provides massive economic improvements as the total refrigeration duty is reduced from an initial 16.29 MW to a much improved 5.1 MW. These improvements will greatly improve the plant economics as operational expenditure will be significantly reduced due to the network improvements. The MER HEN does require extra heat exchangers to facilitate this improved utility usage increasing the number of pre-integration exchangers from 18 to 24. However, this small additional amount of capital expenditure is greatly offset by the energy savings across the plant.

The heat exchanger network introduces additional complexity to the system due to more intricate piping arrangements; however, as discussed, this is offset over the plant's lifetime by the resulting improvements in operating costs. Additionally, it should be stated that for the purpose of control and safety, process to process heat exchangers were carefully considered to only exchange heat between units in closer proximity. The final MER HEN is presented in *Figure 4.3* and the heat exchangers, and their costs are presented in Table 4.4 (the final heat exchanger costs are calculated using the CAPCOST program).

Table 4.4: Summarised Heat Exchanger Table

Heat exchanger	Type	Minimum approach temperature (°C)	Log mean temperature difference (°C)	Duty (kW)	Area (m <sup>2</sup> )	Capital cost (\$)
1	Process-Process	62.62	71.23	18320.0	857.3	154000
2	Process-Process	56.1	82.75	9261.0	373.1	93700
3	Process-Process	78.66	80.82	697.8	28.8	37700
4	Process-Process	104.2	117.97	110.9	3.1	5920
5	Process-Process	79.6	85.88	16230.0	629.8	127000
6	Process-Process	114.5	129.88	15170.0	389.4	95900
7	Process-Process	117	117	21230.0	604.7	123000
8	Process-Process	80.57	86.39	2374.0	91.6	50700
9	Process-Process	78.67	95.47	28470.0	994.0	170000
10	cooling water	23.84	55.04	2113.0	128.0	57200
11	cooling water	7.01	35.98	3012.0	279.0	80600
12	cooling water	40.51	67.37	17330.0	857.3	154000
13	cooling water	22	23.67	3470.0	488.7	109000
14	cooling water	32.3	34.74	19480.0	1869.0	153000
15	cooling water	11.01	41.44	46140.0	3711.0	162000
16	cooling water	7.01	14.82	2984.0	671.0	132000
17	cooling water	34.6	41.61	2453.0	196.5	68400
18	cooling water	7.4	11.31	7186.0	2118.0	136000
19	Process-Process	16.21	27.1	377.2	46.4	41600
20	Process-Process	5.00	9.88	2104.0	709.6	136000
21	Process-Process	12.42	58.78	4790.0	271.6	79600
22	Nitrogen Refrigerant	12.73	22.64	1114.0	164.0	63200
23	Nitrogen Refrigerant	5.7	5.85	4000.0	2280.0	7520
24	Process-Process	123.31	132.24	243.9	6.1	33900
25	Process-Process	5.09	18.4	254.3	46.1	41500
				<b>Total</b>	<b>17,814 m<sup>2</sup></b>	<b>\$2,313,440</b>



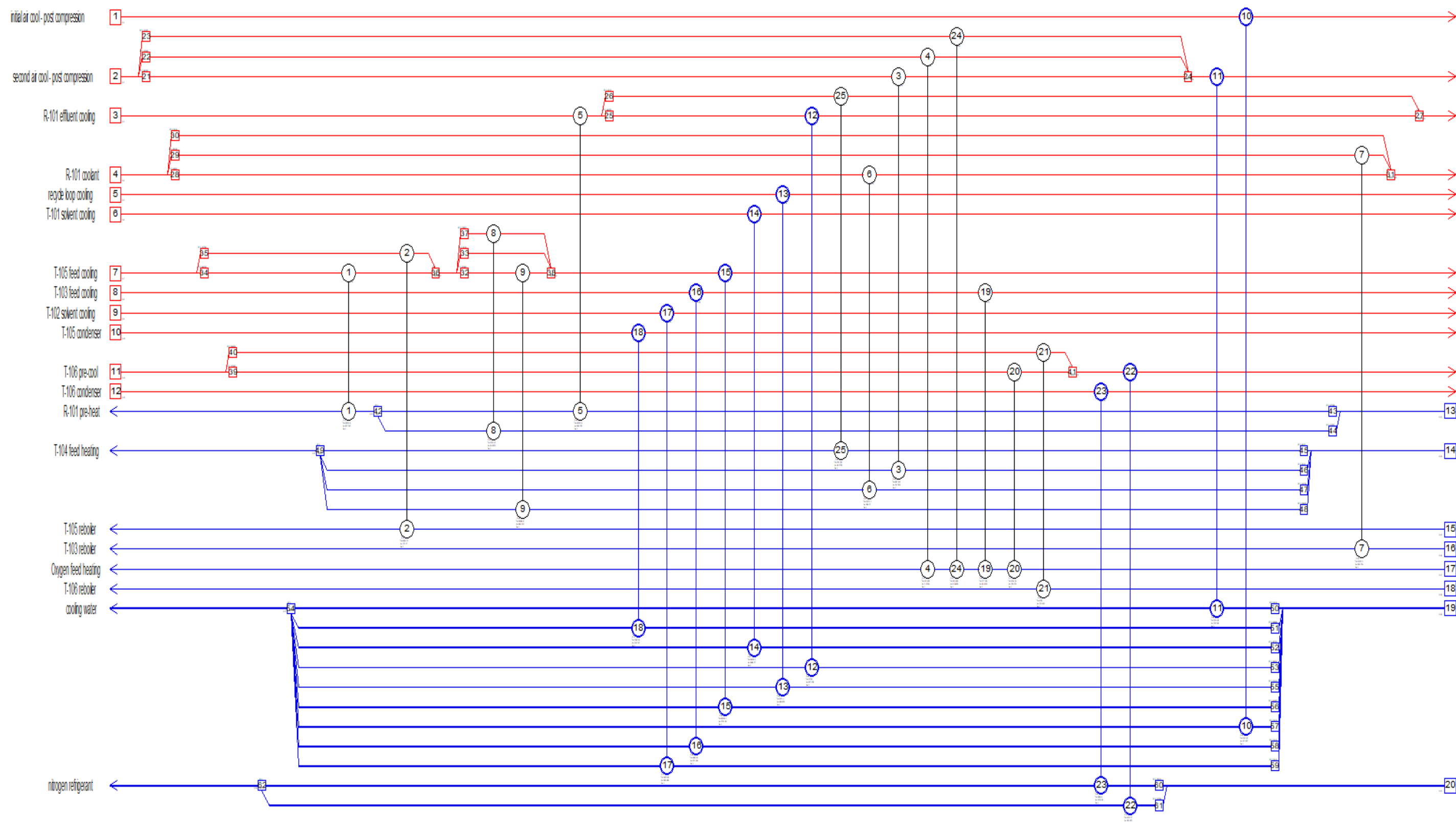


Figure 4.3: Balances Composite curve (red line – hot streams, blue line – cold streams, vertical lines – heat exchangers)

## 5 Detailed Plant Layout

Plant layout represents the arrangement of processing equipment, machinery, piping, buildings and storage tanks within a chemical plant to ensure safe, efficient and cost-effective operations. Safety considerations play an important role in the design and layout of a chemical plant, particularly for hazardous processes like Ethylene Oxide production. They affect the equipment spacing, material flow, emergency systems and regulatory compliance ([Ciricillo, S. \(2019\)](#)). For high-risk processes such as EO production, whose risks and dangers include flammability, toxicity and explosive decomposition, the layout must be laid out and thoroughly designed in a manner that ensures sustainable and accident-free operations. Heuristics, grounded in practical, experience-based guidelines, will be used to simplify and guide complex plant layout decisions. This section delves into the fundamentals of plant layout, the influence of safety considerations and the role of design heuristics in determining the optimal equipment arrangement. The next section will first identify the key process units present in the plant along with the auxiliary buildings.

### 5.1 Key Process Units and Ancillary Buildings

Firstly, the ancillary buildings that were identified are shown in Table 5.1 alongside its justification. The area designated for each building was determined using the following methodology. The area required per person was obtained from a reference and then multiplied by the number of occupants present during peak operational times and is shown for each building. ([Moran, S. \(2017\)](#))

Table 5.1: Area of Ancillary Buildings

Building / Plot	Justification	Area (m <sup>2</sup> )
Office	Used for project management, administrative tasks, and plant operation coordination. Assume 50 employees comprising of engineers, plant managers, and site leaders. Recommended 10 m <sup>2</sup> per employee.	500
Canteen	Designated area for staff meals and breaks, ensuring productivity and compliance with welfare regulation. Assume 50 people at peak time, and 4 m <sup>2</sup> per employee.	200
Control Room	Central hub for monitoring and controlling production operations, ensuring safety and efficiency in ethylene oxide synthesis. Assume 10 employees at peak time and 10 m <sup>2</sup> per employee.	100
Fire Station	Critical for rapid emergency response due to EO's high flammability and toxicity. Assume 10 fire personnel and 6 m <sup>2</sup> per personnel.	60
Security Office	To maintain site safety, control and monitoring to safeguard personnel and hazardous materials. Assume 5 security officers and 7 m <sup>2</sup> per officer.	35
Laboratory	Necessary for quality control, testing raw materials/products, and checking compliance with safety regulations. Assume 20 scientists, technicians and support staff with 15 m <sup>2</sup> per personnel.	300
Medical Centre	Protects the health of employees by offering prompt treatment for chemical exposure or accidents. Assume 15 people at peak operational times, with 15 m <sup>2</sup> per person.	200
Warehouse	Securely store equipment and spare parts, ensuring efficient assembly and maintenance.	550
Workshop	Essential for equipment maintenance, repairs, and fabrication. Assume 10 workers and 20 m <sup>2</sup> per employee	200

Boiler House (Consisting of Flare System)	Provides steam for process heating and sterilisation, necessary for operating units	400
Water Treatment Plant	Treatment of process wastewater to generate high quality cooling water for process cooling.	625
Emergency Assembly Point	Designated secure zone for personnel accountability and evacuation during ethylene oxide leaks or other hazardous events.	100
Car Park	A car park ensures safe, organised employee and visitor parking, reducing hazards and improving site efficiency.	1000
Loading Bay	Ensures secure, compliant, and efficient material handling in high-risk chemical operations	1200

After having determined the area for each of the ancillary buildings, the cross-sectional area for each of the process units was determined. The dimensions of the units were determined from Part 2 of the Design Project and are presented in Table 5.2.

Table 5.2: Dimensions of Process Units

Process Unit	Diameter (m)	Height (m)	Cross Sectional Area (m <sup>2</sup> )
Reactor <b>R-101</b>	10	15	78.5
Cryogenic Distillation Column <b>T-106</b>	2.3	47.1	4.1
Absorption Column <b>T-101</b>	3.7	15.2	10.8
Absorption Column <b>T-102</b>	1.6	8.6	2.1
Desorption Column <b>T-103</b>	1.4	16	1.4
Flash Column <b>T-104</b>	2.7	4.6	5.7
Distillation Column <b>T-105</b>	1.7	27	2.2

Process equipment upstream of the cryogenic distillation column T-106 are grouped together and situated within the air pre-treatment plant with estimated area of 729 m<sup>2</sup>

Having identified the cross-sectional area's for both the process units and ancillary buildings, this will be used to construct both the 2D and 3D Layouts. The next section will identify the storage tanks required alongside its sizing method.

## 5.2 Storage Arrangement for Raw Materials and Products

In ethylene oxide production, maintaining an uninterrupted supply of feedstock and safe storage of finished products is essential due to the continuous nature of the process. Storage tanks are allocated for the following chemicals along with their respective dimensions as listed in Table 5.3.

Table 5.3: Dimension of Storage Tanks

Storage Tank	No. Of Tanks	Diameter (m)	Height (m)	Area (m <sup>2</sup> )
Ethylene Tank	1	17	25.5	227.5
Methane Tank	1	10.7	16.1	89.9
Water Tank	3	10	15	78.5
Ethylene Oxide Tank	1	15.4	23.1	186.5

Oxygen which is produced on-site is not stored due to safety concerns. Storing large volumes of oxygen introduces a significant ignition hazard because of its strong oxidising properties, thereby increasing the risk of fire or explosion. Consequently, oxygen is directly routed to the epoxidation reactor without intermediate storage. Storage tanks for potassium carbonate solvent are also not allocated as the solvent is recovered and recycled entirely in the carbon capture process under normal continuous operation. Additionally, potassium carbonate reserves may be stored in the warehouse as a salt.

Ethylene and methane are stored in cryogenic tanks as liquefied gases (LNG) to improve space efficiency and mitigate the hazards associated with high-pressure gas storage in large-scale facilities. Storing ethylene, methane and ethylene oxide in liquid phase offers economic and safety benefits. Liquefied storage provides significantly higher storage density than gas vessels, thus reducing tank volume and providing better space utilisation. Furthermore, liquefied storage enhances safety by reducing the likelihood of leakage of flammable vapours or vessel rupture resulting from vapour overpressure.

### Sizing Methodology

In terms of storage tank sizing, it is common practice for chemical manufacturing plants to have a minimum storage capacity of 7 days as a buffer against supply chain disruptions. Feedstock storage is sized based on the net input of the process and hence the storage volume of ethylene and methane is determined from their make-up flowrate over the 7-day period. To enhance operational flexibility and safety, a 10% overdesign margin is applied. This accounts for external disturbances such as temperature and pressure fluctuations as well as potential overfilling events. Once the total storage volume is determined, tank dimensions are sized using a height-to-diameter aspect ratio of 1.5:1, following Stephen Hall's rule of thumb for storage vessel design (Hall, S (2020)). According to the API 650 code, LNG tanks can be designed with capacities up to 500,000 m<sup>3</sup>. Given that the calculated storage requirements fall well below this limit, only one storage tank is needed per chemical. For site water storage, a practical approach is taken in the absence of a direct sizing formula. Three water tanks, each with a 10 m diameter and 15 m height are proposed to reliably meet the water demands of the entire facility. The calculated dimensions of the storage tanks are presented in Table 5.3. All the storage tanks are cylindrical and mounted vertically.

### Safety considerations

Ethylene, methane and ethylene oxide are all highly flammable gases, making leak prevention a critical safety priority. To ensure safe storage, all tanks are equipped with gas detection and alarm systems that continuously monitor for potential leaks. Since these substances are stored under pressurised conditions, each tank is fitted with pressure relief valves and rupture discs to provide multiple layers of overpressure protection. Tanks should be constructed from stainless steel for chemical compatibility and corrosion resistance and are often designed with double walls to provide thermal insulation and contain any potential breaches. Additionally, nitrogen blanketing is used to maintain an inert atmosphere within the tank headspace, reducing the risk of ignition and minimising oxygen ingress.

## 5.3 Key Heuristics

Heuristics serve as a general guideline for the arrangement and spacing of plant infrastructure. All infrastructure is situated outdoors to provide natural ventilation and prevent the accumulation of flammable vapour. Plant layout follows a hierarchical approach starting from site layout followed by plot layout.

The process equipment available on-site is divided into two separate plots which are the cryogenic distillation plot and main process plot. The combination of a flammable atmosphere and high-temperature reactor in the main process plot, when located near cryogenic distillation units with elevated oxygen concentrations increases the risk of localised fires and hence necessitates their separation into distinct plots with a minimum distance of 30 m from each other. The same applies for the spacing between process plots and the tank farm to prevent fire hazards from coming into proximity with large quantities of flammable substances in the storage tanks. Literature (Moran, S (2017)) suggests the central location of tank farms in chemical plants as industrial practice. The loading bay is located adjacent to the tank farm for logistical efficiency. As the loading bay handles frequent transfer of flammable liquids, potential ignition is inevitable and requires a safety buffer of 15 m away from the tank farm to prevent a domino effect where a fire outbreak in the loading bay leads to a secondary incident in the tank farm. The control room is placed near the process plots at

a minimum distance of 20 m to balance operational efficiency with safety and accessibility. The proximity between the control room and process plots provides visibility of the process areas and facilitates monitoring while a sufficient distance allows timely evacuation for the control room staff during emergencies. The fire station is located 10 m away from the process plots to allow immediate intervention during fire breakout. Expansion plots are allocated for the process plots and tank farms with an area of approximately 20% of that of the original plot in need of increasing production capacity.

Following the site layout, the process units in each process plot are arranged. Each process unit is contained within a bund wall set at 5 m from the equipment to provide adequate spill containment. The process units are spaced 5 m apart measured from the edges of their respective bund walls to reduce the risk of fire propagation. In the tank farm, adjacent storage tanks are placed 15 m apart for the same reason. (Moran, S (2017))

## 5.4 2D Layout

This section presents the two-dimensional layout of the plant, which illustrates the spatial arrangement of equipment, piping, structures, utilities, and process units within the plot. After having gathered the key dimensions of the process units, ancillary buildings, and storage tanks it was decided to expand the plant area that was initially proposed in Part 1 of the design project to accommodate all structures. Figure 5.1 illustrates the boundaries of the plant at the location, Freeport, Texas indicated by the red lined area. The projected dimensions of the entire plant area are 258 m x 194 m. The detailed 2D plant layout is shown in Figure 5.2.



Figure 5.1: Aerial Photo of Selected Plot

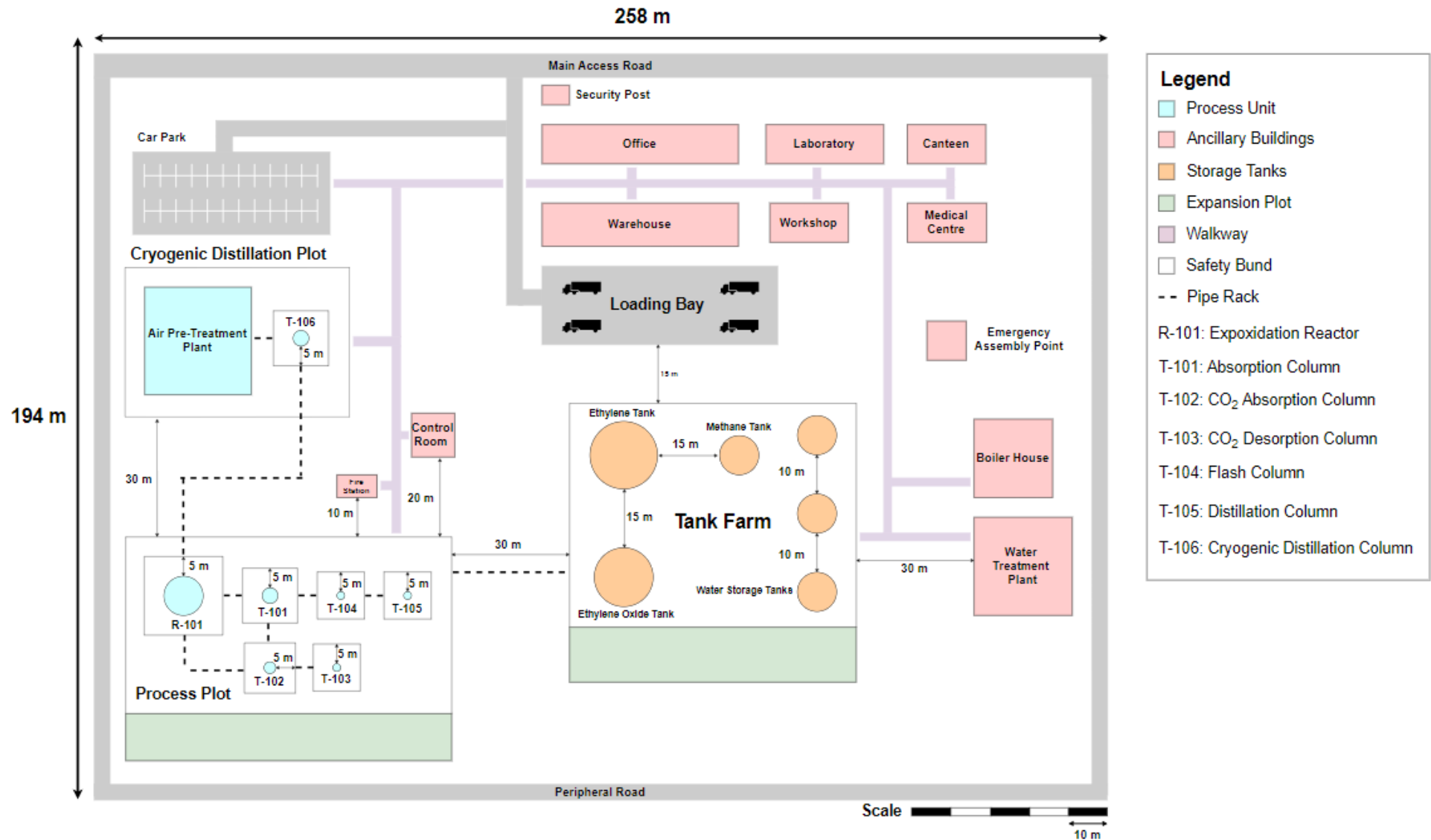


Figure 5.2: 2D Plant Layout



## 5.5 3D Layout

This section presents the three-dimensional layout that represents the physical arrangement of the structures in a virtual space. The 3D Layout was constructed using P5.JS and is presented in Figure 5.4. The side view showing the relative heights of the buildings is shown in Figure 5.3. In both figures, it is worth noting that distillation column T-106 is enclosed inside a cold box which is represented as a cuboid structure.

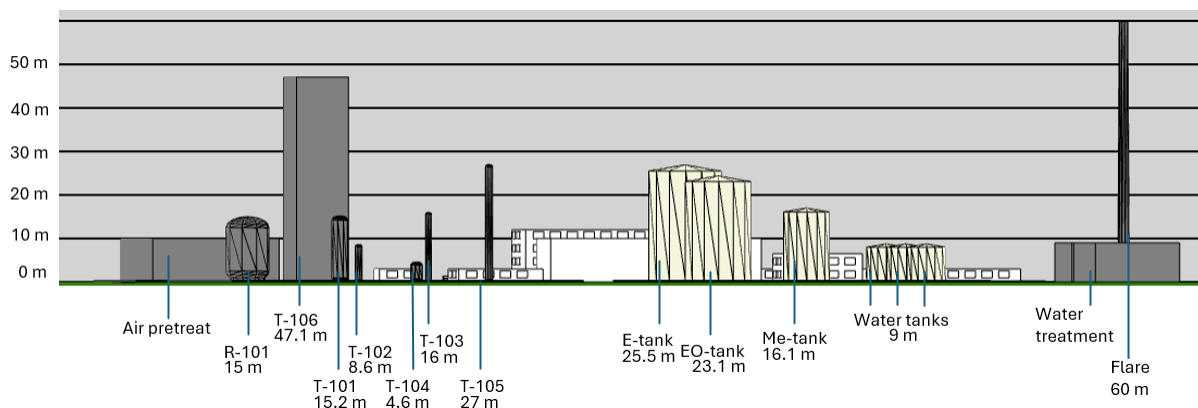


Figure 5.3: Orthogonal Side View of the Plant

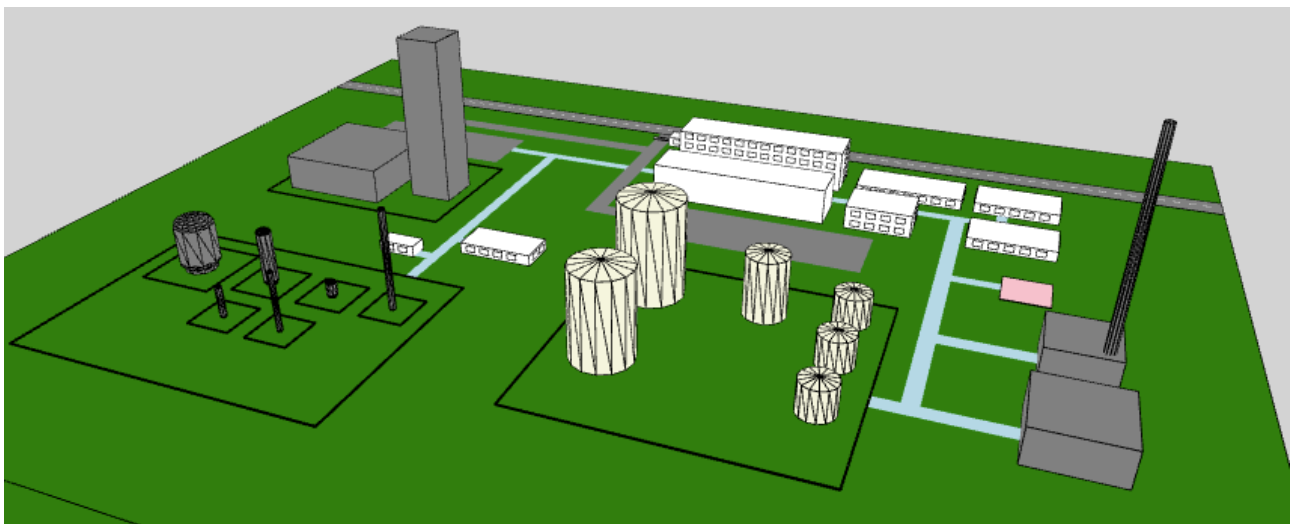


Figure 5.4: Birds Eye View of the Plant

## 6 Sustainability

Ethylene Oxide is a high value chemical that is used in sterilizers, antifreeze, and plastics but its production is energy intensive and hazardous. The sustainable production of EO is crucial to mitigate environmental risks, ensure economic efficiency and contribute positively to society. Environmental risks include that EO is a carcinogen and tight control on its emissions is required. The emission of light gases must also be strictly controlled and sent to a flare system due to the flammability of these gases. The production process emits large amounts of CO<sub>2</sub> which can leave a large environmental greenhouse gas (GHG) footprint. Followed by this, sustainability is crucial for economic viability and efficiency. This includes energy optimization, where sustainable practices including heat recovery can reduce costs. As the process produces byproducts including CO<sub>2</sub>, potentially reusing it for urea production can contribute to a more sustainable circular economy and improve profitability. Environmental, Social and Governance (ESG) compliance may also attract funding from investors and customers alike. The final pillar of sustainability that needs to be considered is the social impact

and this includes worker safety, promoting fair labor conditions, and engaging transparently with local communities. This includes offering fair wages and training opportunities, ensuring robust safety protocols are in place, and minimizing the risks of accidents that could impact surrounding communities. In summary, the sustainable production of ethylene oxide involves striking a balance between social responsibility, economic viability and environmental protection. It contributes to the creation of long-term value for industry and society by lowering emissions, minimising resource use, and encouraging ethical and safe practices. The following section will explore environmental and social sustainability, whilst the economic viability is further explored in detail in Section 10.

## 6.1 Environmental Sustainability

Environmental sustainability refers to the capacity to preserve ecological balance and conserve natural resources in the environment, ensuring the well-being of both the present and future generations. In the context of the production of Ethylene Oxide, this involves minimising the plant's impact on the environment whilst maintaining safe and efficient production. This includes looking at different ways of managing waste from the plant, reducing greenhouse gas emissions, particularly CO<sub>2</sub> as well as controlling the release of toxic EO vapours. The next section looks at the different ways that waste is managed.

### 6.1.1 Waste Management Strategy and Environmental Considerations

Waste management in the EO plant is incredibly important due to the toxic, flammable and volatile nature of some of the species involved. The plant produces gaseous, liquid, and solid waste streams that require careful treatment or recovery to maintain safety, meet environmental regulations, and optimise resource use. Firstly, the waste produced by process units in the plant is identified in Table 6.1.

Table 6.1 Classification and Treatment of Various Waste in EO Plant

Classification	Waste	Source	Use/Treatment
Solid	Spent Catalyst (Silver based catalyst, with alumina support structure)	Reactor <b>R-101</b>	Closed – Loop Regeneration Service
Liquid	Wastewater containing traces of EO	Distillation Column <b>T-105</b>	Treated in wastewater treatment unit onsite
Gas	Nitrogen, Argon gas Mixture	Cryogenic Distillation Column <b>T-106</b>	Recycled as inert gas blanketing for storage tanks
	Hydrocarbon- Rich Purge Stream	Outlet Gas Stream of Adsorption Column <b>T-101</b>	Routed to a PSA for further separation
	Light Gasses	Vapor Distillate Stream of Column <b>T-105</b>	Routed to a Thermal Oxidiser
	CO <sub>2</sub> emissions from Carbon Capture units	Desorption Column <b>T-103</b>	Carbon Capture and stored underground

Following on from the different identification of waste that is produced on site, a more detailed description of how each of the waste is treated is outlined below.

- Treatment and Management of **Solid Waste** (Spent Silver Catalyst)

As outlined in Part 1 of the Design Project, the catalyst that is used in the production of EO in reactor **R-101** consists of silver-based catalyst with an alumina support. Over time the catalyst deactivates due to poisoning, sintering, coking and due to overheating and must be replaced. Due to its valuable metal content and potential toxicity, spent catalyst waste must be handled through a combination of recovery, reuse and safe disposal methods.

Firstly, the spent catalyst is collected and retrieved during scheduled maintenance shutdowns from reactor **R-101**. It is critical that the catalyst is handled in enclosed systems or containers to minimise exposure to airborne particulates and prevent silver loss. Silver, particularly in its oxide form, is highly toxic to aquatic life and may cause long-term environmental harm (Bates, K et al (1995)). Inhalation of dusts can cause irritation and inflammation of the respiratory tract (Bates, K et al (1995)). Appropriate PPE and waste labelling are required to comply with hazardous waste regulations.

After careful collection and handling of the catalyst, the spent catalyst is sent to specialised third – party companies that can extract and refine the silver and recycle or safely dispose of the alumina support. Given the plant's location in Freeport, Texas, the spent catalyst will be sent to *Gladieux Metals Recycling*, a Texas-based company that specializes in recycling spent catalysts and recovering valuable metals such as silver. In particular, they offer closed – loop catalyst programs whereby the recovered silver is used to manufacture fresh catalyst for the plant – streamlining procurement and waste management (Aleon Metals. (2023)). The extraction of the silver done by these third-party companies involve pyrometallurgical or hydrometallurgical recovery. After silver recovery, the silver is used to produce a new batch of EO catalyst, tailored to the reactor specifications of **R-101**. The regenerated catalyst is then transported back to the EO chemical plant at a discounted rate. This treatment method for the spent catalyst was chosen due to the numerous advantages offered by regeneration services. It is sustainable as it promotes circular economy principles by reusing valuable silver metal. It is also cost effective and reduces expenses related to raw material procurement and waste disposal. The last benefit is that there is operational continuity whereby some providers maintain stock or offer rapid manufacturing of regenerated catalyst so that the downtime of **R-101** may be minimised.

The alternative would be to dispose of this spent catalyst in a landfill and utilise primary silver extraction. Silver is a valuable metal, and recovering it helps reduce costs while decreasing dependency on primary silver extraction. Primary silver extraction involves extraction, crushing, milling, smelting and refining all of which are highly energy intensive. The recycling of silver catalysts requires significantly less energy, as the metal is already concentrated and more readily accessible in its chemical form. This reduced energy requirement will lead to a reduction in the carbon footprint, contributing to lower greenhouse gas emissions. Another issue with silver mining is that it often leads to land degradation, deforestation and heavy metal contamination in water and soil. Avoiding this route also helps preserve ecosystems and reduces toxic runoff and habitat destruction. Lastly, the recycling of these catalysts minimises waste and prevents the landfilling of spent catalysts which may contain toxic residues. Instead, the silver is reused in new catalysts, contributing to a more circular economy, reducing hazardous waste generation and promotes resource efficiency.

In summary, the recycling of silver from spent EO catalysts in the closed – loop catalyst programs supports sustainability by cutting emissions, reducing environmental degradation and preserving finite resources making the EO production process greener and more responsible.

- Treatment and Management of **Liquid Waste** (Wastewater containing traces of EO)

After having discussed the keyways of managing the solid, spent catalyst waste the next classification of waste that must be treated is liquid waste, which includes wastewater containing traces of EO from the bottoms of Distillation Column **T-105**. It is typically treated or recovered through a combination of the following strategies, depending on plant design, regulations and cost-effectiveness. This is illustrated in Figure 6.1

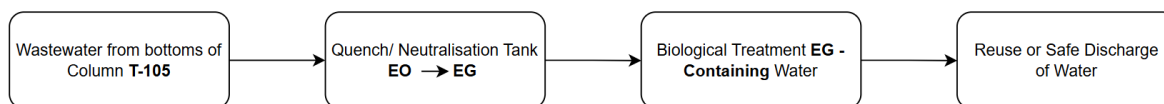


Figure 6.1 Phases of Treatment of Wastewater containing traces of EO

The wastewater is managed through a controlled hydrolysis and biological treatment sequence. Firstly, the treatment process begins with the hydrolysis in a quench/ neutralisation tank. EO as explored in Part 1 of the Design Project, is highly reactive in water and hydrolyses to ethylene glycol. This reaction is promoted in a quench tank to safely degrade residual EO in alkaline conditions through the use of an alkaline such as sodium hydroxide. The reason that the traces of EO is transformed into Ethylene Glycol (EG) is because EO is volatile, carcinogenic and highly toxic to microorganisms used in downstream treatment process.

Followed by the hydrolysis reaction, the mixture containing primarily EG is then directed to a biological treatment unit such as an activated sludge system where EG is biodegraded. This integrated approach ensures safe detoxification of hazardous EO whilst meeting environmental discharge regulations. Based on the quality of the treated water, the effluent is either safely discharged or recycled for further treatment and use in the water treatment section of the plant for use as scrubber make up or cooling water utility.

This waste management method is sustainable as it detoxifies ethylene oxide by hydrolysis and facilitates the safe biodegradation of its by product, ethylene glycol, without producing harmful emissions. It also allows for potential water reuse within the plant, reducing freshwater consumption and minimising environmental impact.

- Treatment and Management of **Gas Waste**

Following on from the management of liquid waste in the EO plant, the next waste that needs to be sustainably and carefully managed is gaseous waste. As outlined in Table 6.1, there are four sources of gaseous waste emitted from the plant. Firstly, the management of the Nitrogen, Argon mixture emitted at the top stream of Cryogenic Distillation Column **T-106** will be discussed.

The EO Plant consists of several storage tanks, as outlined in Table 5.3 which includes an ethylene, methane and ethylene oxide tank. The nitrogen-argon gas mixture vented from the top of cryogenic distillation **T-106** is captured and recycled as part of the inert gas blanketing strategy. Instead of discharging this inert stream into the atmosphere, it is compressed, processed, and diverted for utilisation as a blanketing gas in the storage tanks for ethylene oxide, ethylene, and methane. It eliminates the need for additional industrial nitrogen supply, therefore reducing the plant's environmental footprint and operating costs. The recycled gas creates an inert atmosphere that displaces oxygen and moisture in the vapor spaces of storage tanks, thereby reducing the risk of fire and explosion. This approach aligns with core sustainability principles, including resource circularity, waste reduction and improved process safety.

The next gaseous stream that needs to be treated is the purge stream from the outlet of the gas stream from adsorption column **T-101**. The purge stream contains significant amounts of hydrocarbon (methane, ethylene) alongside some inert (nitrogen). Firstly, gas separation technologies including pressure swing adsorption (illustrated in Figure 6.2) is used to separate the hydrocarbons from the stream and isolate them. This hydrocarbon rich stream is then routed to a thermal oxidiser equipped with heat recovery unit to convert waste gasses into energy, which reduces the overall utility consumption. Meanwhile, the inert rich stream (nitrogen) is recycled for use as inert blanketing for the storage tanks once again. This approach aligns with core sustainability principles, including resource efficiency, waste reduction and energy integration.

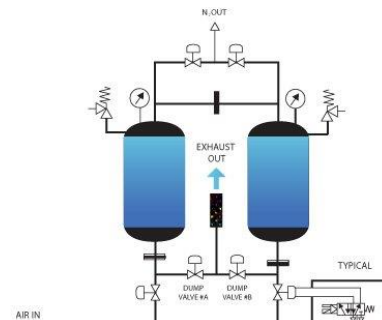


Figure 6.2 PSA Schematic Diagram [Foxolusion. (2022)]

Thereafter, the next gaseous stream that needs to be treated is the light gasses that are vented from distillation column **T-105**. This stream contains predominantly non-condensable light gasses including methane, ethylene, oxygen. This type of waste in industry is typically routed to a thermal oxidiser, whereby hydrocarbons are safely combusted, converting them into less harmful products such as CO<sub>2</sub> and water vapour. While CO<sub>2</sub> is generated, this route significantly reduces the release of high Global Warming Potential (GWP) gasses like methane and ensures plant safety by eliminating flammable or explosive gas mixtures. If feasible, heat recovery systems are integrated to improve the overall energy efficiency of the treatment process.

The final gaseous stream that needs to be treated and managed is the CO<sub>2</sub> that is captured from the carbon dioxide capture units in the plant. The most sustainable approach involves repurposing it for various uses. If feasible, this includes rerouting and using it for urea production (in ammonia plants), CO<sub>2</sub> – enhanced methanol synthesis, mineral carbonation or using it for carbonated beverage (Ali, M (2008)) (Han, P.A. (2021)). This may only be feasible if the plant is located geographically near any one of the following industrial facilities that consumes CO<sub>2</sub>. It helps contribute to a key sustainability principle of circular economy, whereby waste is turned into product. However, this may not be a feasible route and hence an alternative must be considered. If there is no nearby Carbon Capture and Utilisation (CCU) opportunities available, the CO<sub>2</sub> captured will be compressed, dehydrated and sent to geological storage. Typical storage methods include deep saline aquifers, depleted oil and gas reservoirs, and enhanced oil recovery (Amin Izadpanahi et al (2024)). This also contributes to the sustainability of the EO plant as long term sequestration prevents atmospheric release, reducing the plants carbon footprint.

Having identified and evaluated different methods of managing all the waste emitted from the plant, the next section will look to conduct a comprehensive Life Cycle Assessment in order analyse CO<sub>2</sub> emissions.

## 6.2 Life Cycle Assessment (LCA)

Life Cycle Assessment (LCA) is a method for methodically examining the environmental implications of product, process or service during its full lifecycle from raw material extraction to production, use and disposal (Nickel, L. (2024)). The system boundary for this study will follow the “Cradle to Gate” approach and is further explored in the next section. The purpose of the LCA is to identify ‘hot spots’ in the EO plant, effectively areas where there are high environmental impacts and identify opportunities for improvement. The LCA will be conducted in accordance with the ISO methodology, which involves defining the project's goal and scope, performing an inventory analysis, carrying out an impact assessment, and concluding with an interpretation of the results. The impact assessment is carried out using the *CCaLC2* software. Hence firstly, the assumptions and limitations of the study is explored in the next section.

### 6.2.1 Assumptions and Limitations

Before following the LCA methodology, there are several assumptions that have been made and limitations with the study conducted. Hence, the assumptions made for this study and their respective limitations are outlined in Table 6.2.

Table 6.2 Assumptions and Limitations with LCA Methodology

Assumption	Description/ Justification	Limitation
Normal Operation Only	LCA excludes start – up, shut-down, and commissioning phases. Focus is only on steady state, continuous operation	LCA won't capture spikes in emission and resource use; Hence GWP and resource metrics underestimated
Electricity Usage limited to turbomachinery	Only major process equipment, including pumps and compressors are considered. Electrical consumption for lighting, control systems, etc. are neglected.	Underestimates the total electricity demand and related GWP impact
Domestic water usage neglected	Water used for domestic purposes Only process-related water consumption (e.g. cooling) is included.	Slight underestimation of water footprint
Refrigeration Compression Power omitted	Energy required for refrigeration compressors (e.g. in cryogenic distillation) is excluded.	Underestimates energy demand and GWP of Cryogenic Distillation Unit
Cooling Water Energy Consumption	Cooling Water flowrate is derived from flowrate and time for one functional unit. Power Requirement estimated using a correlation of 0.0009 MJ/kg	It is a simplified method; does not consider temperature lift or site-specific cooling system efficiencies.
Outdated database CCaLC2	Environmental burden data for utilities are based on older database dating back from around 2007 -2010	May not reflect updated grid mixes, technology improvements or regional changes. Hence accuracy is limited

It is acknowledged that there are several limitations in the methodology and assumptions adopted, including the exclusion of start up phases, reliance on outdated environmental datasets, and simplified utility estimations. The analysis will proceed and the results gathered should be interpreted with these considerations in mind. Despite these limitations, the study still provides valuable insights into the relative sustainability performance of the process. With this in mind, the next section will proceed with the first stage of the LCA which includes defining the purpose and scope of the study.

### 6.2.2 Goal Scope and Definition

The purpose of the LCA study on the EO plant is to identify and evaluate the environmental impacts associated with the production of EO from raw material extraction through to the factory gate. This boundary is known as the “Cradle-to-Gate” approach as it doesn't take into account use and disposal of the EO product. These phases were excluded from the study to avoid introducing excessive assumptions that could compromise accuracy. The study will focus on identifying key environmental hotspots in the raw material and production processes, providing data to inform energy integration strategies and sustainability improvements within the EO production plant. It will also look at the impact of Process Integration on the environmental impact. With the purpose of the study established, the next section will begin with defining a functional unit to ensure a consistent basis for comparison.



### 6.2.3 Functional Unit

A functional unit is defined as a quantified reference of the product's function used to calculate environmental impacts (Backes, J.G (2023)). It provides a consistent basis for comparing environmental impacts across the life cycle stages of EO production. In the context of this study, the functional unit will be defined as *1000 kg of EO produced*. This mass based functional unit follows industry standards and allows for scalable results. Following on from the identification of the functional unit, the transportation across site is identified in the following section.

### 6.2.4 Transport

Transportation refers to the movement of materials, products or components at any stage of the production of EO's life cycle and the environmental impacts associated with it. Within the system boundary defined in this study, transportation is limited to the delivery of raw materials to the ethylene oxide (EO) production site. The supplier and type of transportation for each of the raw materials are all summarised in Table 6.3.

Table 6.3: Raw Material, Supplier and Type of Transportation

Raw Material	Supplier	Type of Transportation
Ethylene	DOW Chemicals	Underground Pipeline
Methane	Kinder Morgan	Underground Pipeline

It is important to note that as ethylene and methane are supplied via underground pipelines by the respective suppliers, their transportation environmental burden will not be assessed in the LCA study as there is none. Following on from the identification of transportation, the LCA methodology follows with conducting an inventory analysis.

### 6.2.5 Inventory Analysis

Inventory analysis is the second phase of the LCA process whereby all the inputs and outputs are quantified (materials, energy, emissions, etc.) associated with the EO production process across the cradle to gate boundary. Firstly, the input (raw material) was identified and quantified in terms of kg FU<sup>-1</sup> and shown in Table 6.4. After that the utility requirement of the plant before heat integration was quantified and tabulated in Table 6.5. Finally, the product and waste coming out from the EO plant per functional unit was quantified in Table 6.6.

Table 6.4: Input of LCA Study (Raw Material Flowrate Per Functional Unit)

Input	Flowrate (kg FU <sup>-1</sup> )
Ethylene	955.3
Methane	152.3
Water (Make Up)	36356.1

Table 6.5: Utility Requirements Before Heat Integration

Utility	Power (MJ FU <sup>-1</sup> )
Electricity (Electricity Mix, USA)	4071.4
Steam (From Natural Gas)	21761.4

Table 6.6: Output of LCA Study (Product and Waste Flowrate Per Functional Unit)

Output	Flowrate (kg FU <sup>-1</sup> )
Wastewater	7690
EO Product	1039.6
Cryogenic Waste	2977.1
Purge	218.9

Light Gas Waste	36.4
Captured Carbon Dioxide	389.7

After outlining and conducting the inventory analysis, the LCA proceeds in the next section with an impact assessment and interpretation of the results.

### 6.2.6 Impact Assessment and Interpretation

Impact assessment and interpretation is the final stage of the LCA methodology. The impact assessment involves translating raw data from inventory into environmental impacts. As a CO<sub>2</sub> emission analysis is to be conducted to determine the carbon footprint of the plant, the impact category that will be used in this analysis is Global Warming Potential (GWP) and is expressed in kg CO<sub>2</sub> – equivalent FU<sup>-1</sup>. Following the impact assessments, the results will be interpreted to identify the main contributors (hotspots) to the overall environmental impacts.

Firstly, Figure 6.3 illustrates the GWP of the 2 different stages consisting of Raw Material and Production Stage

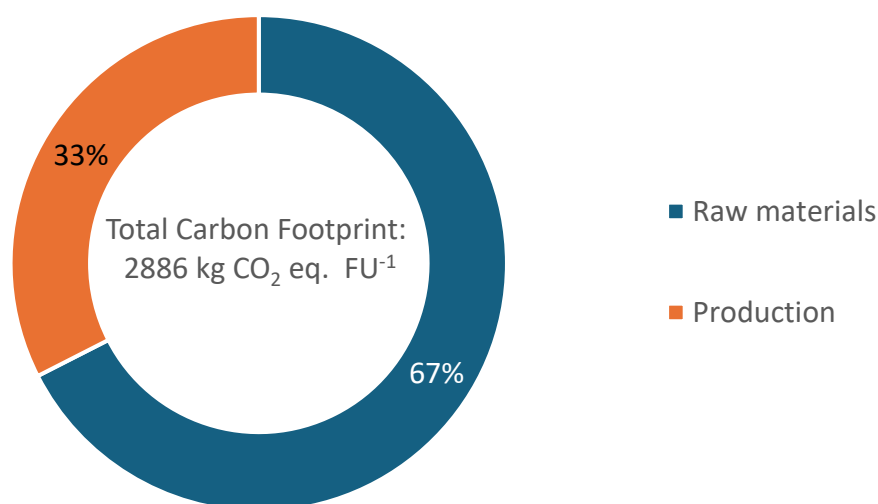


Figure 6.3: Total Carbon Footprint Across EO Site

Figure 6.3 illustrates the breakdown of the total carbon footprint of the EO production process, which amounts to 2886 kg CO<sub>2</sub> eq. per functional unit (FU<sup>-1</sup>). The GWP is distributed across two primary life cycle stages: Raw material acquisition and production. As illustrated above:

- Raw Materials Contribute to 67% of the total GWP (Approximately 1933.6 kg CO<sub>2</sub> eq. FU<sup>-1</sup>)
- Production Accounts for 33% of total GWP (Approximately 952.4 kg CO<sub>2</sub> eq. FU<sup>-1</sup>)

This distribution indicates that raw material sourcing is the dominant contributor to the carbon footprint, over twice that of the production phase. This makes sense in the context of EO synthesis because the main feedstocks, ethylene and methane are produced using energy intensive procedures. From a sustainability perspective, these insights suggest that carbon reduction strategies should primarily target the raw materials stage. Hence a further breakdown of the raw materials is conducted in the next section.

### Raw Material Analysis

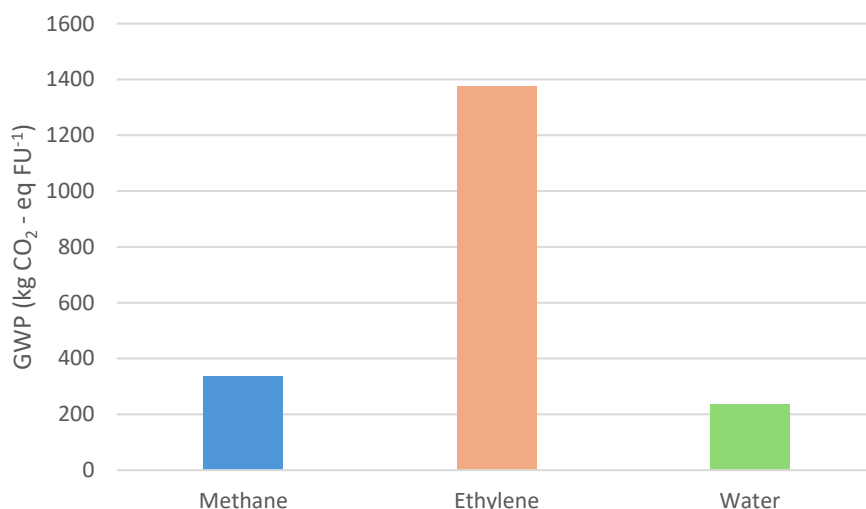


Figure 6.4: Global Warming Potential of Raw Materials

The carbon footprint of raw materials used in ethylene oxide production was evaluated using CCalc to identify the primary contributors to global warming, enabling targeted mitigation efforts. Figure 6.4 shows that ethylene has a significantly higher carbon footprint than methane and water, accounting for 70.6% of the total emissions from raw materials. This high impact is attributed to the use of conventional ethylene produced via steam cracking which is a highly energy-intensive process associated with substantial greenhouse gas emissions. Despite its environmental impact, the decision to use conventional ethylene was supported by the Multi-Criteria Decision Analysis (MCDA) conducted in Part 1 of the Design Project, which highlighted its wide availability, cost-effectiveness and secure supply. The ethylene is sourced from a nearby petrochemical plant, ensuring a reliable and uninterrupted feedstock supply which is critical for stable plant operations. Additionally, conventional ethylene remains economically favourable compared to lower-emission alternatives. However, as an environmentally responsible manufacturer, the plant should actively explore and adopt lower-carbon ethylene sources when such alternatives become economically viable.

## CO<sub>2</sub> Emission Analysis

This section aims to conduct a CO<sub>2</sub> emission analysis to determine the effect of heat integration on the EO process. Heat integration involves looking at opportunities for process-to-process heat recovery as discussed in Section 4 to reduce utility requirements and hence lead to an overall lower carbon footprint. Following heat integration, the system becomes a threshold problem in which only cold utilities are required – cooling water and refrigerant – are required as highlighted in Section 4. As with the before analysis, the GWP was assessed using CCalc2 tool. The methodology for inputting the energy requirements is outlined below.

Before heat integration, both hot and cold utilities were required across the various sections of the plant. All hot utility demand was in the form of steam. For each process section, the steam requirement was quantified in MJ per functional unit and entered into CCalc2 accordingly. Cold utility consisted of cooling water and refrigerant. As the refrigerant cycle was not designed and the compressor requirements were unknown, it was excluded from the analysis and hence only cooling water was included as highlighted in the assumptions and limitations section.

Since CCalc2 does not allow direct input of cold utility, the energy requirement associated with cooling water was estimated indirectly. The mass of cooling water required per functional unit was calculated by multiplying the cooling water flowrate by the time required to produce one functional unit (1000 kg of EO). The mass was then multiplied by a correlation factor of 0.0009 MJ per kg of water (Pontes, R.F.F (2022)), yielding the equivalent power requirement. This correlation factors comes from the indirect energy consumption associated with the circulation of cooling water, primarily due to the operation of pumps and auxiliary equipment.

After heat integration, the remaining cooling water demand for each process section was summed. Using the same correlation factor, the corresponding energy requirement, now in the form of just electricity was calculated. The comparative GWP results for both pre – and post integration scenarios are presented in Figure 6.5.

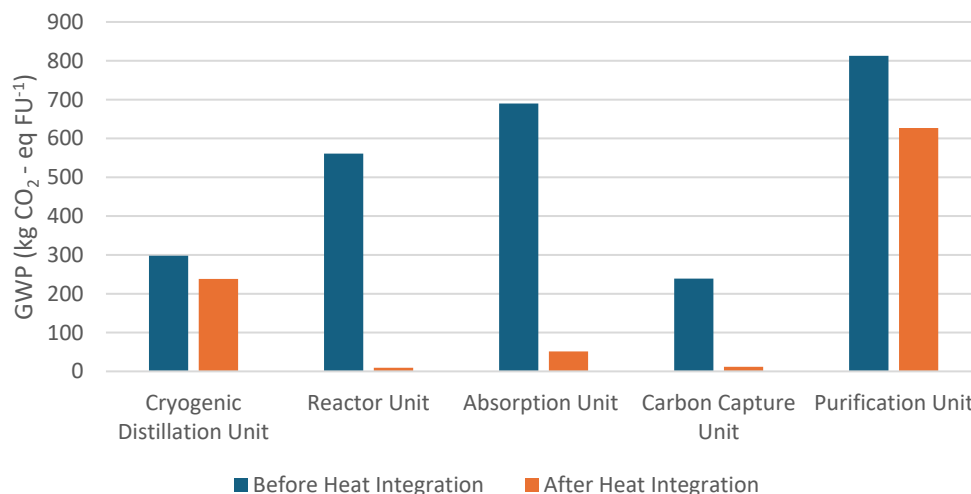


Figure 6.5 - Global Warming Potential of EO Processing Units Before and After Heat Integration

Figure 6.5 illustrates the GWP of the various process units before (highlighted in blue) and after (highlighted in orange) heat integration. The figure demonstrates a consistent reduction in GWP across all units following the implementation of heat integration, demonstrating its effectiveness in reducing carbon emissions.

The Absorption unit showcases the most significant reduction in GWP, reducing from approximately 700 kg CO<sub>2</sub> - eq FU<sup>-1</sup> to under 100 kg CO<sub>2</sub> - eq FU<sup>-1</sup>. This sharp decline indicates that the absorption process had previously relied heavily on utility, which were significantly reduced through heat recovery.

Similarly, the reactor and carbon capture units exhibit a significant decrease in GWP, nearing zero post – integration. This indicates that these units made substantial use of the redistributed excess heat within the process, significantly reducing their reliance on external utilities.

The cryogenic distillation unit also showcases a moderate reduction in GWP from about 290 kg CO<sub>2</sub> - eq FU<sup>-1</sup> to about 230 kg CO<sub>2</sub> - eq FU<sup>-1</sup>. Despite still achieving a reduction, it is the second largest contribution to the GWP and hence a major contributor to overall emissions. One limitation of this analysis is the exclusion of compression power, as the refrigeration cycle for the cryogenic distillation unit was not designed in Part 1. As a result, the electricity required for compression was not considered, which likely underestimates the actual GWP, especially considering the high energy demand of refrigeration systems.

The EO purification unit shows a less pronounced decrease, from around 800 kg CO<sub>2</sub> - eq FU<sup>-1</sup> to 620 kg CO<sub>2</sub> - eq FU<sup>-1</sup>. Despite achieving a reduction, it remains to be the largest contributor to GWP across the whole plant, due to its reliance on cold utility and less efficient heat integration opportunities.

Hence the result of heat integration yielded an overall 63.9 % reduction in GWP, highlighting the impact of heat integration in mitigating environmental burdens.

In summary, the data supports the conclusion that heat integration significantly lowers GWP across most EO units. However, units like the EO purification unit may require further optimization strategies to enhance their environmental performance.

## 6.3 Social Sustainability

Social sustainability involves safeguarding and improving the wellbeing, equity and rights of individuals and communities, both in the present and future generations. Social sustainability in the EO production plant is promoted by enforcing rigorous health and safety standards, engaging with the local community and ensuring the operation generates fair economic opportunities without compromising one's wellbeing. The first aspect of social sustainability that will be explored is the occupational health & safety of the workers and local communities.

### 6.3.1 Occupational Health & Safety Measures

Ethylene Oxide is classified as a toxic, flammable and potentially carcinogenic compound. One of the core sustainability priorities is that all workers on the EO plant is protected. First and foremost, the plant will follow and implement the Occupational Safety and Health Administration (OSHA) Process Safety Management (PSM) standards for all the hazardous chemicals which include process hazard analysis, operating procedures, mechanical integrity and emergency planning.

To ensure this, there are several measures in place, which are illustrated in Table 6.7:

Table 6.7: Occupational Health and Safety Measures in Place in EO Plant

Safety Measure	Justification
Fixed and Portable EO gas detectors	Enables early detection of EO leaks to prevent toxic exposure and explosion risk
Automatic Emergency Shutdown (ESD) Systems	Immediately isolates critical equipment during high – risk scenarios to prevent escalation
Explosion – Proof Instrumentation and Wiring	Minimizes ignition sources in areas with EO vapor presence
Double – Walled Piping and Leak Containment	Prevents EO release into the environment and improves maintenance safety
Mandatory use of PPE including SCBA in designated zones	Protects personnel from inhaling EO vapors, which are acutely toxic and carcinogenic
Regular Process Hazard Analyses (PHA) under OSHA PSM guidelines	Identifies and mitigates potential failure modes before incidents occur
Routine Health Screening and long – term EO exposure monitoring	Enables early detection of EO – related health effects and complies with occupational exposure limits
Emergency Response Plans and Community Drills	Prepares personnel and nearby communities for prompt action in case of accidental EO release
Comprehensive EO handling and spill response training	Ensures staff know how to safely handle EO and respond to leaks or exposure incidents

After having identified all the safety measures that are in place to ensure the occupational health of all workers on site, the next section will look at another aspect of social sustainability, - community health and environmental justice.

### 6.3.2 Community Health & Environmental Justice

As the plant is located in Freeport, Texas there are very many residential areas that are located close to the plant and thus the plant must operate in a way that minimizes health and environmental risks to the surrounding communities. Therefore, specific initiatives have been implemented to mitigate against this and are outlined below.

The highly industrialized Brazoria County, where the Freeport EO plant is located, has high levels of industrial air pollutants. The first initiative includes putting into place extensive monitoring and control measures at the fence line (outer perimeter of plant) and in nearby neighborhoods due to the

cariogenic risks of EO and other hazardous air pollutants (methane, ethylene). The adjacent petrochemical site, (DOW Freeport) performs bi weekly perimeter sampling for volatile organics using Environmental Protection Agency (EPA) Method 325 (DOW Freeport (2025)). Building on this practice, the plant will be putting into place ambient EO monitors to look for any fugitive or stack emissions along the fence line and close to sensitive receptors (community centers, schools).

Next, the plant will engage and implement air dispersion modelling to confirm that offsite EO concentrations remain significantly below EPA's long term acceptable cancer risk threshold of 100 ppt. The model helps predict where and how EO and other pollutants will travel under different wind and weather conditions. Through simulation of both routine and worst-case scenarios, the plant can evaluate whether EO levels in nearby residential areas remain below the EPA's long term cancer risk threshold of 100 ppt.

Another initiative includes ensuring public access to air monitoring data vis dashboards or annual community reports. Clear and transparent communication of environmental data fosters public trust and supports informed community engagement. Online dashboards allow residents to view recent air quality from fence line monitors in real time. Annual reports with plain language summaries help translate complex technical data to information that is accessible and understandable to the community. This is an important initiative especially in an area like Freeport, Texas whereby residents may have concerns regarding air quality and emissions resulting from cumulative industrial exposure.

The final initiative that will be implemented is focusing and promoting environmental justice. It is an integral part of the plant's risk management. The Freeport community has a high proportion of minority and low-income residents (over 55% Hispanic and 55% low income), indicating potential vulnerability (Freeporttx.gov. (2024)). These communities are more often vulnerable to environmental risks. To address this, the EO plant will use EPA's Environmental Justice (EJ) Screen and state EJ mapping tools to identify local pollution burdens and demographic factors. This initiative ensures that the facility's operations do not disproportionately impact vulnerable populations and helps foster greater transparency, accountability, and equitable decision-making in environmental planning. Having discussed the key plans and initiatives taken for community health and environmental justice, the next section considers stakeholder engagement and transparency.

### **6.3.3 Stakeholder Engagement & Transparency**

Another important aspect of social sustainability is stakeholder engagement and transparency. This is especially important in Freeport, Texas as residents have heightened sensitivity to industrial risks due to past regional incidents, including the 2019 Port Neches TPC explosion (CSB (2022)). This caused widespread evacuation and health concerns amongst the community. Consistent, ongoing and open communication with stakeholders enhances trust and ensures that the operation aligns with the community expectations. The stakeholder initiatives include the formation of a Community Advisor Panel (CAP) with representatives from neighborhood associations, local schools, hospitals and municipal agencies. This is important as it encourages two – way dialogue between plant leadership and community and ensures local perspectives influence decision making particularly around safety and expansion.

Next, quarterly town halls are established to discuss plant performance, environmental results, and planned expansions. This includes public forums where plant managers share updates, respond to questions and gather direct feedback from residents. This is key as it promotes transparency and accountability surrounding the EO plant and fosters public confidence in operational safety and environmental compliance. It highlights the plants commitment to responsible practices.

Finally, essential EPA Clean Air Act documents should be summarized and will be made easily accessible online and in local libraries or government offices. This is to ensure regulatory compliance and a proactive stance on safety and provides reassurance that the plant is prepared for

emergencies. Following these initiatives, the final aspect of social sustainability that is considered is local employment and economic impact.

### **6.3.4 Employment & Local Economic Impact**

The EO production process is capital and labor intensive, which allows for opportunity for local employment. Hence the first initiative involves commitment to local hiring for operators, technicians and administrative roles. This includes from regions including Freeport and surrounding areas in the Brazoria County including Lake Jackson, Clute and Angleton. Prioritizing hires from the local region and town helps anchor the plant workforce in the local economy. This is important as it reduces unemployment and provides economic stability in industrial communities. It also enhances workforce reliability and community support by drawing from the regional labor base.

The next initiative that will be implemented is providing apprenticeship and training programs in collaboration with Brazosport College, aligning curriculum with plant needs. Partnerships and collaborations with local institutions such as Brazosport college to develop tailored coursework and hands on training that match real – world plant roles help build a pipeline of skilled local talent. This reduces dependency on out of town hires and enhances youth employability.

Finally, a paid internship scheme will be implemented for high school and university students, with priority to applicants from underrepresented or low-income backgrounds. This enables and provides meaningful, paid experience that introduces students to industry early. This is important as it expands pathways to technical careers for historically underrepresented groups in STEM, promoting diversity, equity and inclusion within the workforce.

## **6.4 Design Choices for More Sustainable EO Production Plant**

The implementation of carbon capture units on site has significantly reduced carbon emissions in the production stage. Nevertheless, the sustainability performance of the plant can be further enhanced through the incorporation of energy-focused design measures to reduce the carbon footprint associated with the plant's power and utility requirements. The proposed measures are on-site renewable electricity generation and flare gas recovery through Combined Heat and Power (CHP) systems. These measures align with circular economy principles by positioning the plant as an environmentally responsible manufacturer, well-prepared to adapt to future market demands and policy shifts toward low-carbon industrial practices.

The integration of solar photovoltaic panels offers a strategic opportunity to reduce the carbon footprint associated with electricity consumption. By generating a portion of the plant's power demand through renewable energy, reliance on grid electricity typically generated from fossil fuel sources is significantly reduced. This not only mitigates greenhouse gas emissions but also improves energy resilience and reduces long-term operational costs. Implementing solar infrastructure aligns with the plant's long-term sustainability goals and offers environmental and economic co-benefits.

Secondly, the plant's design can be further improved through the utilisation of vent gases in a Combined Heat and Power (CHP) system. Instead of solely flaring excess gases which contribute directly to greenhouse gas emissions, these gases can be combusted in a CHP unit to simultaneously generate electricity and steam. This approach transforms a waste stream into a valuable energy source. Although steam may not be needed internally due to heat integration strategies, any surplus can be exported to nearby facilities or sold to utility providers, thereby generating additional revenue while improving the overall energy efficiency of the plant.



## 7 HAZOP and Safety Considerations

### 7.1 Process Hazard Analysis (PHA) Outline:

To ensure the safe operation of a chemical production process, it is essential to conduct thorough Process Hazard Analyses (PHA). There are various methodologies available, such as LOPA, HAZID, or HAZOP, with the choice often depending on the specific stage of the process design. During the early stages of design, as covered in Part 1, a preliminary Hazard Analysis (HAZAN) was performed to identify key areas of risk and potential safety concerns.

Hazard analysis is generally approached in progressive stages, as outlined in the IChemE six-stage hazard study model (Enis (2011)). In the exploratory and flowsheet development phases, initial assessments of process safety and integrity can be carried out using techniques like HAZID or HAZAN — both of which serve to highlight significant hazards early in the design. Once the process advances to a more detailed design stage, and comprehensive documentation such as P&IDs becomes available, more rigorous hazard evaluation techniques, like HAZOP, can be systematically applied (Enis (2011)).

### 7.2 HAZOP Aims:

HAZOP (Hazard and Operability Study) is a rigorous, systematic approach to identifying potential hazards and operational issues within a process. It aims to focus on cause-based analysis to uncover all credible risks that could impact personnel, the environment, or facility assets. By examining process flows, equipment configurations, and control systems in a structured, team-based setting, HAZOP ensures that risks are thoroughly assessed, and appropriate mitigation measures are developed. (Li (2020))

Since HAZOP addresses deviations from normal operating conditions, it demands an in-depth understanding of the process. To achieve this, a multidisciplinary team with extensive knowledge of the chemical industry and the specific process under review was assembled, ensuring comprehensive coverage of all potential scenarios. (Li (2020))

### 7.3 HAZOP Methodology:

This section will outline the methodology used to conduct the HAZOP study, this is a multistate process which allows for the meticulous identification of hazards and facilitates the development of targeted actions to reduce associated risks. This is achieved by following the procedure laid out Rossing et al in 'A Functional HAZOP Methodology'. (Rossing (2010))

#### 7.3.1 Deviation matrix

The first step in conducting this PHA is to summarise the vast range of potential hazards that can occur in the form of a deviation matrix. The deviation matrix gives a guideword and a property which combine to form a deviation from normal operation. The deviations are then used to allow those carrying out the HAZOP to think of potential causes for the deviation and their consequences. Some properties and guidewords are explained here for clarity: utilities refers to the use of external heating or cooling utilities; AWA stands for 'as well as', meaning another event occurs along with the intended function; PO stands for 'part of', meaning the cause is a function of another deviation; REV refers to 'reverse' and OTH refers to 'other'.

#### 7.3.2 Risk and Action

For each identified deviation, it is essential to systematically determine and document all potential causes and consequences. Once the consequences of a hazard are understood, the next step is to assess the level of risk it presents. Risk can be evaluated, quantified, and represented as a Risk Matrix, as shown in Table 7.1, this matrix was developed based on those presented in literature (Baybutt (2015), Marhavidas (2019), Hao (2022)). Based on the assessed risk level, appropriate safety measures can then be defined. These measures, outlined as recommended actions, are intended to be implemented following the completion of the HAZOP to enhance process safety.

Table 7.1: Risk Level analysis table.

Severity of Event	Likelihood				
	Extremely Unlikely ( $< 10^{-6}$ /yr)	Very Unlikely ( $10^{-6}$ to $10^{-4}$ /yr)	Unlikely ( $10^{-4}$ to $10^{-2}$ /yr)	Possible ( $10^{-2}$ to 1/yr)	Probable ( $> 1$ /yr)
Catastrophic			Intolerable Risk	Intolerable Risk	Intolerable Risk
Major				Intolerable Risk	Intolerable Risk
Serious	Acceptable Risk				Intolerable Risk
Significant	Acceptable Risk	Acceptable Risk			
Minor	Acceptable Risk	Acceptable Risk	Acceptable Risk		

### 7.3.3 Dividing the P&ID

It is advisable to split the overall process into individual areas or nodes. Each node has a specific design intent different to other sections of the process. This modular approach allows for the minimisation of the probability that a potential hazard will be missed as more focus can be applied to individual aspects of the process in contrast to viewing the process as an overall unit.

The overall P&ID for the process can be divided into a number of areas, the key area that will be investigated in this section is the reactor area (Area 2). This was identified as a key area of potential safety concern in the **Part 1** HAZAN study, this is due to the high pressure and temperature requirements in this part of the process compared to upstream and downstream processing, for this reason a rigours HAZOP will be conducted to identify all key hazards and deviations in this area and subsequent actions and improvements can be made, so safe operation can be guaranteed.

## 7.4 Conducting HAZOP

This section of the report outlines the findings of the HAZOP, detailing identified hazards, their associated risks, existing safeguards, and recommended actions for risk reduction. Emphasis has been placed on ensuring that all foreseeable deviations from normal operating conditions have been considered, and that appropriate layers of protection are either in place or proposed to maintain the highest standards of safety and regulatory compliance

## STUDY TITLE: HAZOP Study of Ethylene Oxide Production Plant

AREA: 2 of 6

SECTION DESCRIPTION: Reactant feed to Reactor (R-101)

TEAM COMPOSITION: all members

SECTION IMAGE:

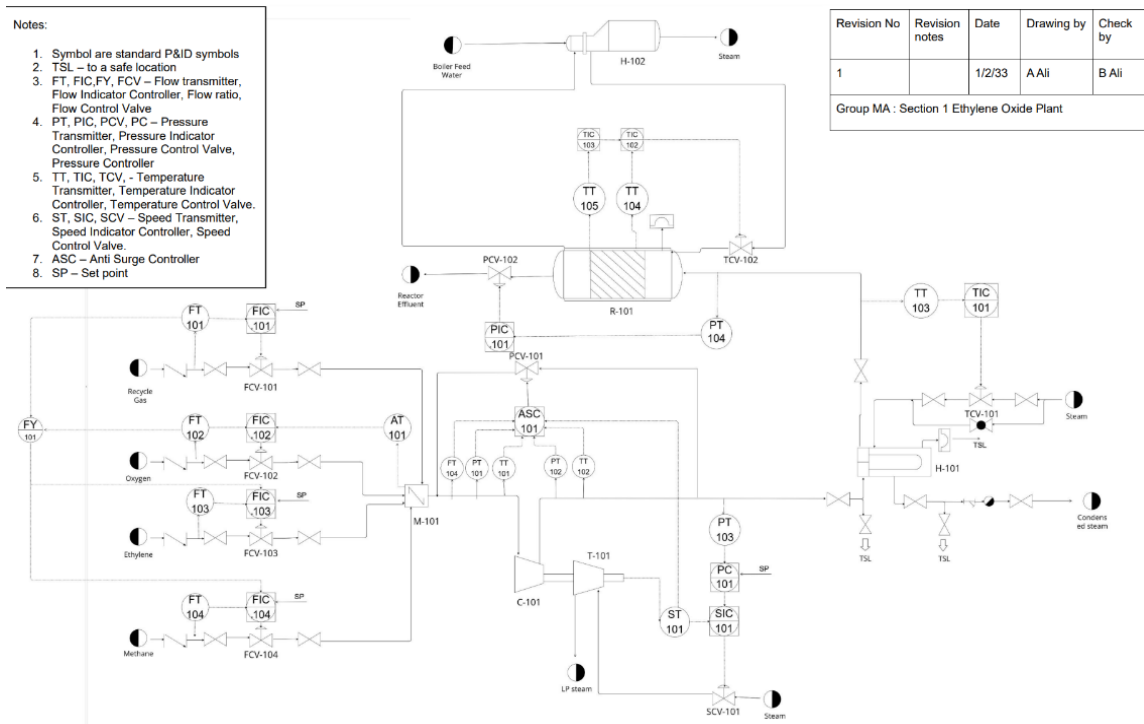
## DESIGN INTENT:

The reactor is designed to produce 150,000 to 170,000 tonnes per year of ethylene oxide (EO) through the partial oxidation of ethylene using oxygen, with methane added as an inert to reduce flammability risks. The process involves highly exothermic reactions, requiring careful thermal management to optimize EO selectivity (target  $\geq 80\%$ ) while minimising complete combustion to  $\text{CO}_2$ . A multi-tubular fixed-bed catalytic reactor with a silver-based catalyst is selected for its efficiency and suitability for heat removal via an external cooling medium.

Operating conditions are typically in the range of 200–300°C, selected to be at 210 °C and 15–30 bar selected to be 18.5 bar, with a high ethylene-to-oxygen ratio to favour selective oxidation. Methane serves to dilute oxygen concentration and prevent explosive mixtures. The design prioritizes process safety, heat control, and conversion efficiency (25–35% per pass), with integration into downstream quenching, absorption, and recycle systems to ensure continuous, safe, and cost-effective EO production.

## Notes:

1. Symbol are standard P&ID symbols
2. TSL – to a safe location
3. FT, FIC, FY, FCV – Flow transmitter, Flow Indicator Controller, Flow ratio, Flow Control Valve
4. PT, PIC, PCV, PC – Pressure Transmitter, Pressure Indicator Controller, Pressure Control Valve, Pressure Controller
5. TT, TIC, TCV, TC – Temperature Transmitter, Temperature Indicator Controller, Temperature Control Valve
6. ST, SIC, SCV – Speed Transmitter, Speed Indicator Controller, Speed Control Valve
7. ASC – Anti Surge Controller
8. SP – Set point



	NO	MORE (HIGH)	LESS (LOW)	AWA	PO	REV	OTH
Flow	X	X	X		X	X	
Pressure		X	X		X		X
Temperature		X	X		X		
Corrosion / Erosion		X					
Contamination		X			X		
Concentration		X	X				
Maintenance	X	X					X
Utilities	X	X					
Electrical	X	X			X		

Deviation	NO.	Possible causes	Consequences	Existing controls	Risk level	Actions required
<b>FLOW</b>						
<b>No flow</b>	1.1.1	<ul style="list-style-type: none"> <li>Control valves <b>FCV-101, FCV-102, FCV-103, FCV-104</b> failed closed or blockage</li> <li>Non return valve or isolation valve around <b>FCV-101, FCV-102, FCV-103, FCV-104</b> failed closed or blockage</li> <li>Control loop failures, of <b>(FIC101, FT101, FY101), (FIC102, FT102, FY102), (FIC103, FT103, FY103), (FIC104, FT104, FY104), AT101</b></li> </ul>	Flow of necessary feed into reaction system will be reduced or totally stopped. This could either completely inhibit desired reaction, favour unwanted side reactions or create dangerous atmospheres. This could reduce profitability due to either accumulation of undesired products or damage downstream equipment. If methane flow (the inert species) is stopped oxygen concentration could increase leading to the surpassing of flammability limits which could lead to dangerous fires or explosions.	Existing flow transmitters ( <b>FT-101, FT-102, FT-103, FT-104</b> ) can signify to operators any variation in flow of a given species. Additionally, the composition analyser <b>AT-101</b> will give indication to variations from normal conditions.	Intermediate risk	Regular maintenance of valves and control systems.
	1.1.2	<ul style="list-style-type: none"> <li>Pipe blockages</li> <li>Pipe rupture</li> </ul>	Similar consequences are present as seen in 1.1.1, however pipe blockages reducing flow can lead to overpressure and subsequent explosion. Following on ruptures in pipe, leading to complete loss of flow lead to dangerous reagents or products leaking into plant facility. This could cause toxic or flammable environment. Ethylene oxide is toxic to breathe and there are many flammable components.	N/A	Acceptable risk	Ensure pipe network is regularly checked and maintained. Ensure proper ventilation system.
	1.1.3	<ul style="list-style-type: none"> <li>Failure of <b>C-101</b>, or <b>T-101</b></li> <li>Valve <b>SCV-101</b> failure</li> </ul>	This means that the required pressure driving force cannot be generated, so flow of reagents will be stopped, and necessary pressure of reactor cannot be maintained. This will lead to reduced reaction rate or total inability to carry out reaction.	Pressure transmitter, <b>PT-103</b> , controlling steam flowrate regulates pressure of inlet stream to <b>R-101</b> .	Intermediate risk	If expenditure can be justified auxiliary compressor could be installed. Proper maintenance and inspection schedule to address issues before complete equipment failure.
<b>No flow (part of utilities)</b>	1.1.3	<ul style="list-style-type: none"> <li>Blockage In <b>H-101</b></li> <li>Shell or tube rupture in <b>H-101</b></li> <li><b>TCV-101</b> fails closed or corresponding isolation and drain valves</li> <li>Drain valves could fail open</li> </ul>	This would lead to no heat transfer to process fluid, so necessary reaction temperature will not be met. If heating fluid is blocked and cannot flow, pressure build up of steam will occur potentially leading to explosion, also temperature limits of material can be met.	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-101</b> )	Intolerable risk	Regular maintenance of utility systems and add additional pressure relief value in the case of pressure build up.
	1.1.4	<ul style="list-style-type: none"> <li>Blockage In <b>H-102</b></li> <li>Shell or tube rupture in <b>H-102</b></li> <li><b>TCV-102</b> fails closed, or corresponding isolation and drain valves</li> <li>Drain valves could fail open</li> </ul>	This would lead to no heat removal from reactor, due to exothermic reaction, temperature would continue to increase, hence there is a potential for a runaway reaction and thermal meltdown of the reactor.	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-102</b> )	Intolerable risk	Regular maintenance of utility systems and add additional pressure relief value in the case of pressure build up.
<b>Less flow</b>	1.2.1	<ul style="list-style-type: none"> <li>Control valves <b>FCV-101, FCV-102, FCV-103, FCV-104</b> <b>partial blockage</b></li> <li>Non return valve or isolation valve around <b>FCV-101, FCV-102, FCV-103, FCV-104</b> <b>partial blockage</b></li> <li>Control loop malfunction of <b>(FIC101, FT101, FY101), (FIC102, FT102, FY102), (FIC103, FT103, FY103), (FIC104, FT104, FY104), AT101</b></li> </ul>	Flow of necessary feed into reaction system will be reduced. This could either inhibition of desired reaction, favour unwanted side reactions or create dangerous atmospheres. This could reduce profitability due to either accumulation of undesired products or damage downstream equipment. If methane flow (the inert species) is reduced oxygen concentration could increase leading to the surpassing of flammability limits which could lead to dangerous fires or explosions.	Existing flow transmitters ( <b>FT-101, FT-102, FT-103, FT-104</b> ) can signify to operators any variation in flow of a given species. Additionally, the composition analyser <b>AT-101</b> will give indication to variations from normal conditions.	Acceptable risk	Regular maintenance of valves and control systems.

## Part 3

## Sustainable Production of Ethylene Oxide

Group MA (2025)

	1.2.2	<ul style="list-style-type: none"> <li>Partial blockage of pipe works</li> <li>Small leak occurs in pipe system</li> </ul>	Similar consequences are present as seen in 1.2.1, however pipe blockages reducing flow can lead to increased vapour velocity potentially increasing erosion. Following on leaks in pipes, leading to loss of flow lead to dangerous reagents or products leaking into plant facility. This could cause toxic or flammable environment. Ethylene oxide is toxic to breathe and there are many flammable components.	N/A	Acceptable Risk	Ensure pipe network is regularly checked and maintained. Ensure proper ventilation system.
	1.2.3	<ul style="list-style-type: none"> <li>Malfunction in of C-101, or T-101</li> <li>Valve SCV101 partial blockage</li> </ul>	This means that the required pressure driving force cannot be generated, so flow of reagents will be reduced, and necessary pressure of reactor cannot be maintained. This will lead to reduced reaction rate and non-optimal pressure.	Pressure transmitter, <b>PT-103</b> , controlling steam flowrate regulates pressure of inlet stream to <b>R-101</b> .	Intermediate risk	If expenditure can be justified auxiliary compressor could be installed. Proper maintenance and inspection schedule to address issues before complete equipment failure.
	1.2.4	<ul style="list-style-type: none"> <li>R-101 Bursting disk opens and is not closed</li> <li>PCV 102 fails</li> </ul>	This will reduce overall flow through reactor due to potential leaks into cooling system, this could contaminate utility supply. The reactor pressure reduction could favour different reaction reduced production of desired produce reducing profitability.	N/A	Intolerable risk	Add isolation system around R-101 to immediately cease reaction if dangerous atmosphere is forming, this can allow for engineers to safely address issues.
Less flow (part of utilities)	1.2.5	<ul style="list-style-type: none"> <li>Partial blockage in <b>H-101</b></li> <li>Shell or tube leak in <b>H-101</b></li> <li><b>TCV-101</b> partially blocked or corresponding isolation and drain valves, drain valves could partially open</li> </ul>	This would lead to reduced heat transfer to process fluid, so necessary reaction temperature will not be met. If heating fluid is blocked and cannot flow, pressure build-up of steam will occur.	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-101</b> )	Intermediate risk	Regular system checks and install valve position indicator.
	1.2.6	<ul style="list-style-type: none"> <li>Partial blockage in <b>H-102</b></li> <li>Shell or tube leak in <b>H-102</b></li> <li><b>TCV-102</b> partially blocked or corresponding isolation and drain valves, drain valves could partially open</li> </ul>	This would lead to minimised heat removal from reactor, due to exothermic reaction, temperature would continue to increase. If temperature is not maintained, isomerisation will occur rather than epoxidation.	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-102</b> )	Intermediate risk	Regular system checks and install valve position indicator.
More Flow	1.3.1	<ul style="list-style-type: none"> <li>Malfunction of feed control systems, Control loop malfunction of (<b>FIC101</b>, <b>FT101</b>, <b>FY101</b>), (<b>FIC102</b>, <b>FT102</b>, <b>FY102</b>), (<b>FIC103</b>, <b>FT103</b>, <b>FY103</b>), (<b>FIC104</b>, <b>FT104</b>, <b>FY104</b>), <b>AT101</b></li> </ul>	Flow of given species can increase. This could either inhibition of desired reaction, favour unwanted side reactions or create dangerous atmospheres. This could reduce profitability due to either accumulation of undesired products or damage downstream equipment. If oxygen flow is increased concertation could increase leading to the surpassing of flammability limits which could lead to dangerous fires or explosions. If all species flowrates increase, the system could potentially be overwhelmed and not operate properly in terms of pressure and heat transfer equipment.	Existing flow transmitters ( <b>FT-101</b> , <b>FT-102</b> , <b>FT-103</b> , <b>FT-104</b> ) can signify to operators any variation in flow of a given species. Additionally, the composition analyser <b>AT-101</b> will give indication to variations from normal conditions.	Acceptable risk	Regular maintenance of valves and control systems.
Reverse Flow	1.3.2	<ul style="list-style-type: none"> <li>Failure of non-return valve (NRV)</li> </ul>	This could lead to potential back flow of a mixture of components contaminating feed supply, leading to dangerous reactions in storage containers or overflow/pressure if NRV fails completely.	N/A	Acceptable Risk	Regular maintenance of valve and piping system.
<b>PRESSURE</b>						
Less Pressure	2.1.1	<ul style="list-style-type: none"> <li>Leakage occurring at valve in system</li> <li>Isolation valve not properly closed</li> </ul>	This could reduce operating pressure of reactor meaning that undesired side reactions could become more favourable. Additionally puts additional	N/A	Intermediate risk	Regular maintenance of valve and piping system.

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		<ul style="list-style-type: none"> <li>Pipe leakage or rupture</li> </ul>	stress on compressor to maintain pressure driving force.			
	2.1.2	<ul style="list-style-type: none"> <li>Malfunction or failure of <b>C-101</b></li> </ul>	This will lead to no flow system and high pressure of reactor (1.5-3 MPa) cannot be reached, similar consequences present as <b>2.1.1</b>	<b>PT-103</b> can indicate fluctuations in pressure.	Intermediate risk	If expenditure can be justified auxiliary compressor could be installed. Proper maintenance and inspection schedule to address issues before complete equipment failure.
	2.1.3	<ul style="list-style-type: none"> <li>Failure of reactor pressure controls system (<b>PCV-102, PIC-101, PT-104</b>)</li> </ul>	High pressure of reactor (1.5-3 MPa) cannot be reached, similar consequences present as <b>2.1.1</b>	N/A	Intermediate risk	This could be solved with built in redundancy due to high pressure operation. Additionally independent safety system could allow for worker independent emergency shutdown
More Pressure	2.2.1	<ul style="list-style-type: none"> <li>Malfunction in control of <b>C-101</b></li> </ul>	This would lead to reactor feed entering at a higher pressure, potentially overwhelming the reactor pressure control systems, leading to dangerous overpressure, greater than design stresses.	Reactor pressure controls system ( <b>PCV-102, PIC-101, PT-104</b> ) <b>PT-103</b> , can indicate fluctuations in pressure.	Intolerable risk	If expenditure can be justified auxiliary compressor could be installed. Proper maintenance and inspection schedule to address issues before complete equipment failure.
	2.2.2	<ul style="list-style-type: none"> <li>Blockage in valve or pipe throughout the system</li> </ul>	This will cause buildup of pressure at point in pipe which could subsequently lead to an explosion leaking hazardous materials around plant area.	Pressure transmitters throughout system.	Acceptable risk	Regular maintenance of valve and piping system.
	2.2.3	<ul style="list-style-type: none"> <li>Failure of reactor pressure controls system (<b>PCV-102, PIC-101, PT-104</b>)</li> </ul>	This will cause buildup of pressure within reactor which could subsequently lead to an explosion leaking hazardous materials around plant area. Additionally high temperature and heavy construction materials could lead to particularly dangerous explosion	N/A	Intolerable risk	Build in redundancy into reactor pressure control.
More Pressure (Part of more Temperature)	2.2.4	<ul style="list-style-type: none"> <li>Failure in utility system, insufficient cooling</li> </ul>	This could lead to increased temperature in piping system or reactor, this will lead to expansion of gases components hence overpressure and potential explosion could occur.	Pressure and temperature transmitters throughout system, linked to heat exchanger control.	Intolerable risk	Add pressure relieve valves on pipes that could experience potential overpressures.
TEMPERATURE						
More Temperature	3.1.1	<ul style="list-style-type: none"> <li>Failure in <b>H-102</b> (shell or pipe rupture of leak, <b>TCV-102</b> failure, surrounding isolation and drain valve failure, along with bruising disc failing open)</li> </ul>	This would lead to no heat removal from reactor, due to exothermic reaction, temperature would continue to increase, hence there is a potential for a runaway reaction and thermal meltdown of the reactor.	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-102</b> )	Intolerable risk	Temperature indicators installed at multiple points throughout the system, emergency shut off system connected to feed controllers into the system as temperature reaches dangers height.
	3.1.2	<ul style="list-style-type: none"> <li>Failure in control of <b>H-102</b></li> </ul>	See 3.1.1	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-102</b> )	Intolerable risk	See 3.1.1
Less Temperature	3.2.1	<ul style="list-style-type: none"> <li>Failure in <b>H-101</b> (shell or pipe rupture of leak, <b>TCV-101</b> failure, surrounding isolation and drain valve failure, along with bruising disc failing open)</li> </ul>	This would lead to no heat transfer to process fluid, so necessary reaction temperature will not be met. If heating fluid is blocked and cannot flow, pressure build up of steam will occur potentially leading to explosion, also temperature limits of material can be met.	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-101</b> )	Intolerable risk	See 3.1.1
	3.2.2	<ul style="list-style-type: none"> <li>Failure in control of <b>H-101</b></li> </ul>	See 3.2.1	Drainage systems and bursting disk located on heat exchanger will reduce likelihood of overpressure. Additionally, temperature control regulates flow ( <b>TIC-101</b> )	Intolerable risk	See 3.1.1
CORRSION/EROSION						



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More Corrosion	4.1.1	<ul style="list-style-type: none"> <li>Improper maintenance and construction such as connecting dissimilar metals when replacing parts or not fastening them properly. Dissimilar metals may be in contact if the valves are made from a different metal (affects all valves and pipes in this node).</li> </ul>	This will cause galvanic corrosion, leading to weak points in the system which will not be able to withstand necessary pressures and flows that are required.	N/A	Acceptable risk	Ensure proper investigation is conducted into material selection, take particular care if element must be replaced to consider material selection.
More Erosion	4.2.1	<ul style="list-style-type: none"> <li>Partial blockage or closure of any valve in system, increasing fluid velocity</li> </ul>	Increased fluid velocity will erode internals of piping system, leading to abrasion or erosion of walls. This will lead to weak points in the system which will not be able to withstand necessary pressures and flows that are required.	Flow controls and pressure controls can be used to control vapour velocity	Acceptable risk	Maintain pipe work to avoid obstructions.
	4.2.2	<ul style="list-style-type: none"> <li>Malfunction in compressor control increasing velocity in subsystem</li> </ul>	See X.1.2	Compressor control system (PT-103, PC-101, SIC-101, ST-101)	Acceptable risk	N/A
CONTAMINATION						
More contamination	5.1.1	<ul style="list-style-type: none"> <li>Feed impurities present in inlet streams</li> </ul>	This could lead to catalyst poisoning in the reactor, reducing activity in turn requiring replacement of the catalyst. Additionally, impurities in the feed could cause side reactions, for example excess water could lead to the formation of ethylene glycol in the reactor. Impurities in feed could lead to additional stress on	N/A	Acceptable risk	Filter feed before enters system, ensuring proper pretreatment is conducted to remove impurities.
More contamination (part of erosion)	5.1.2	<ul style="list-style-type: none"> <li>Increased erosion leading to particulate flow from pipe internals in system</li> </ul>	Solids suspended in feed inlets could lead to increased rates of erosion in pipework and damage C-101.	N/A	Acceptable risk	Filter on gaseous inlets
CONCENTRATION						
More concertation	6.1.1	<ul style="list-style-type: none"> <li>Ratio control failure</li> <li>Inlet feed blockage</li> </ul>	If oxygen concertation is increased flammability limits can be reached which could lead to a potential explosion in presence of ignition source. If other regents' concentration increase reaction kinetics could be effected either increasing rate, leading to the potential for runaway reaction where cooling cannot accommodate increased temperature. Conversely if the concertation of the inert methane is increased this could completely suppress the reaction.	Indicators FT-101 – FT-104 can be used to interpret flow into system as well as composition controller ASC-101. These can be used to identify fluctuations in feed conditions.	Intolerable risk	In case of control failure system should be flooded with an inert, this means a quench system could be added to eliminate any flammable atmospheres
Less concertation	6.2.1	<ul style="list-style-type: none"> <li>Ratio control failure</li> <li>Inlet feed blockage</li> </ul>	Similar issues in terms of flammability, and reaction kinetics see x.1.1	Indicators FT-101 – FT-104 can be used to interpret flow into system as well as composition controller ASC-101. These can be used to identify fluctuations in feed conditions.	Intolerable risk	In case of control failure system should be flooded with an inert, this means a quench system could be added to eliminate any flammable atmospheres.
MAINTAINANCE						
High Maintenance	7.1.1	Excessive maintenance leads to extended shut down of plant area.	With extensive shut down times, yearly plant production rates cannot be met, hence profitability and reparation will be affected.	N/A	Acceptable risk	This can be minimized through effective communication, preventing engineers from duplicating maintenance efforts and by providing training on proper maintenance procedures.



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Low/no Maintenance	7.2.1	Area is not regularly checked and maintained leading issues not getting identified or propagating.	If this area is not maintained to satisfactory standards, checks will not be able to identify issues, so prolonged shutdowns will be required leading to issues seen in <b>X.1.1</b>	N/A	Acceptable risk	This can be minimized through effective communication, preventing engineers from duplicating maintenance efforts and by providing training on proper maintenance procedures.
<b>ELECTRICAL</b>						
No electricity	8.1.1	Power cut to the building.	This would lead to all control and alarm equipment requiring electricity to fail. This would cause the process to continue dangerously without control or supervision.	N/A	Intermediate risk	Back-up generator for process. SIS system not connected to mains power supply
No electricity (part of) More electricity.	8.2.1	Power surge to equipment.	If there is a surge in power this could lead to a fuse blowing in any electrical equipment, which would lead to lack of control of system	N/A	Intermediate risk	Monitor electrics of the building.
<b>MIXING</b>						
No mixing	9.1.1	Failure of <b>M-101</b>	Feed components will not be well mixed when entering the reactor this could lead to a reduction in reaction rate or formation of hot spots when entering <b>R-101</b> .	Composition analyser <b>AT-101b</b> , could give indication of feed mixture.	Intermediate risk	N/A
Less mixing	9.2.1	Ineffective mixing in <b>R-101</b> , due to blockage or flowrate reduction	See <b>X.1.1</b>	Less likely to due to plug flow arrangement	Intermediate risk	N/A

## 8. P&ID and cross section pumping

The section to be analysed is the pipeline connecting the gaseous outlet of absorption column T-101 and the gaseous inlet of absorption column T-102.

### 8.1 Piping and pumping considerations

Before the compressor the pipes must be able to withstand the operating pressure of C-101 with at least a 10% safety margin. This marks a pressure of 23.1 bar. The minimum required schedule for this would be 22.3 and is then increased to the next standard stainless-steel schedule of SCH40s. Stainless steel is required as ethylene oxide is corrosive as are the water vapours in the presence of oxygen.

To keep the gas velocity between the standards of  $20 \text{ m s}^{-1}$  and  $30 \text{ m s}^{-1}$  (PhcpPros (2020)), the required pipe diameter leaving T-101 for a SCH40s pipe is DN850 with a gas velocity of  $27 \text{ m s}^{-1}$ . The pipe diameter after the compressor continuing along the main recycle path remains DN850 as the purge and carbon removal pipes are significantly smaller. The pipe split from the main recycle path to feed to the carbon dioxide absorption column must be a size DN300 pipe with a gas velocity of  $23.3 \text{ m s}^{-1}$ .

With 14m vertical descent leaving T-101 and a minimum of 15 m horizontal, the pipe length between the two columns is taken at 30 m, with 20 m being before the compressor and the remaining 10 m after the compressor. Assuming the pipe split towards the carbon columns occurs at the boundary bund for T-102, there are 25m in the DN 850 pipe and 5 m in the DN300 pipe to be considered for pressure losses. (Enerpac (2019)) Fittings and bends are considered in the K values for the pressure drop. A summary of all the pipe fittings are illustrated in Table 8.1

Table 8.1 - Pipe fittings

Fitting	K value	Number present in DN850	Number present in DN300 pipe section
Turns	0.3	5	0
Valves	0.15	3	3
Control valves	0.05	1	1
T junction flow through	0.2	4	3
T junction corner	1	0	1
Sudden entrance	0.5	1	0
Sudden exit	1	0	1

Accounting for the pressure drop over pipe length, the fanning friction factor is given by the equation below:

$$\frac{1}{\sqrt{f}} = -3.6 \log \left( \left( \frac{\varepsilon/D}{3.7} \right)^{1.11} + \frac{6.9}{Re} \right) \quad \text{Equation 8.1}$$

The total pressure drop is then found by incorporating the fanning friction factor, fittings and change in height.

$$\Delta P = \rho g \left( f \frac{4L}{D} \frac{u_i^2}{2g} + \sum_i K_i \frac{u_i^2}{2g} + \Delta h \right) \quad \text{Equation 8.2}$$

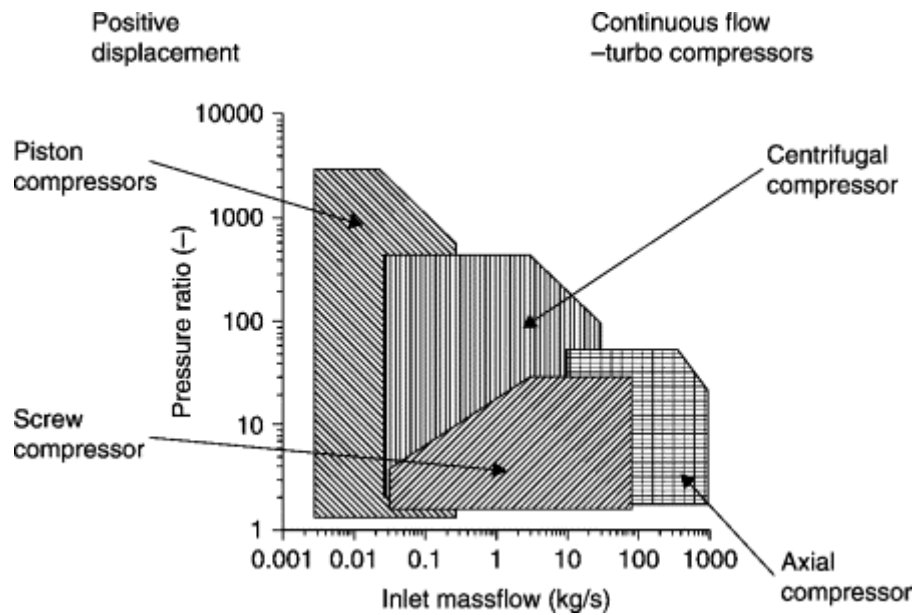


Figure 8.1: Compressor operating regions graph (Bradshaw, C.R. (2013))

The pressure gain for the gas required by the compressor C-103 is found to be 0.86 bar. Due to the high throughput of this compressor (242 kg/s) and low pressure ratio, an axial compressor would be the most suitable as seen in figure 8.1. (Bradshaw, C.R. (2013))

8.2 P&ID

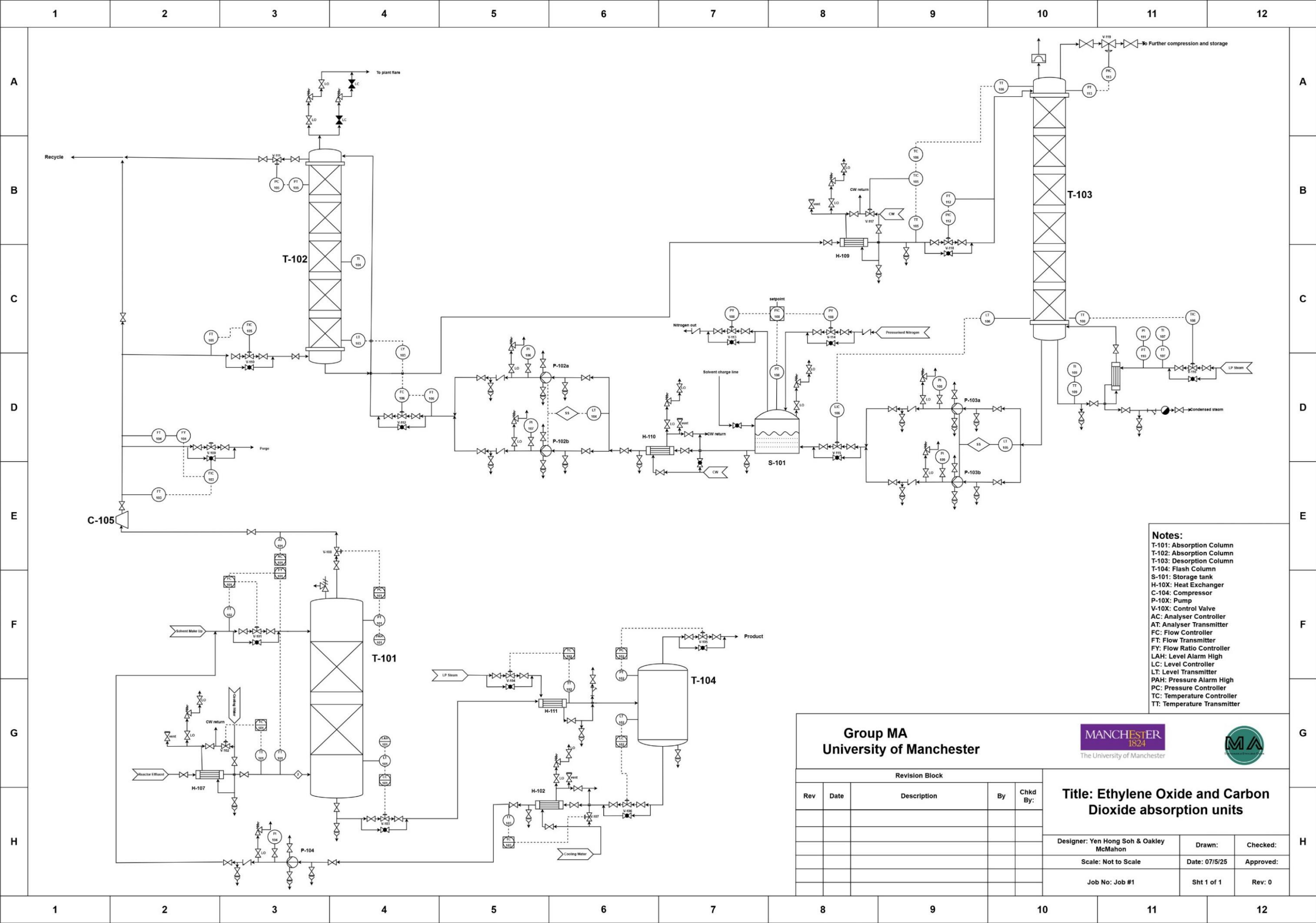


Figure 8.2: P&ID of Ethylene oxide and carbon dioxide absorption sections

## 9 Operating Considerations

Operating an ethylene oxide production facility requires strict adherence to engineering, environmental and safety regulations. This section outlines the key operational phases throughout the plant's lifecycle.

### 9.1 Plant Commissioning

Commissioning is a systematic process aimed at verifying that all installed equipment and systems perform in accordance with the design intent and operational requirements. The primary objective is to ensure that the facility is safe, functional and ready for operation, hence enabling a smooth handover from the contractor to the plant owner. This process also serves to identify and resolve any issues prior to startup. The key stages involved in the commissioning procedure are outlined below. (OJ automation (2024))

#### 9.1.1 Planning

The planning phase is the foundation of the commissioning process as the success of the entire commissioning process relies heavily on the thoroughness of the planning stage. In this phase, the scope, objectives and timelines of the project are defined. First, a comprehensive commissioning plan is developed which outlines the roles and responsibilities of all stakeholders including project managers, contractors and engineers. Key documents such as the commissioning schedule, risk assessments and quality assurance plans are also created in this phase.

#### 9.1.2 Procurement

Process equipment and materials are sourced according to the specifications outlined in the planning stage. Emphasis is given to items with long lead times to ensure timely delivery to site. Factory Acceptance Testing (FAT) is a crucial part of this phase as it involves testing the purchased equipment at the manufacturer's facility before delivery to site. This ensures that the purchased equipment meets the required standards and specifications. Any discrepancies identified during FAT can be addressed promptly, preventing delays while saving time and resources down the line.

#### 9.1.3 Inspection

After completing the installation of procured equipment along with its associated mechanical, electrical and control systems, the installed equipment is to be inspected before the introduction of process fluids into pipelines and vessels. Table 9.1 presents an inspection checklist to identify and rectify any deficiencies before proceeding to the next phase of commissioning.

Table 9.1: Pre-commissioning Inspection Checklist

Category	Item	Status
Personnel and Safety	Permit to work approved by plant owner.	
	All personnel have completed their medical assessment and are equipped with personal protective equipment (PPE).	
	Sufficient first aid kits and fire extinguishers are available on site.	
	All safety and alarm systems are functional.	
	Commissioning test area is free of debris and cordoned off.	
Process Equipment	Internal components are clean and free from debris.	
	Trays in distillation columns are installed at correct levels and intact.	
	Correct type and height of packing in absorption column.	
	Correct height and placement of catalyst bed in reactor.	

	Leak test performed on distributor trays in columns.	
	Correct installation of pressure relief valves.	
	Drains and vents are connected to correct safe locations.	
Heat Exchangers	Piping and tubes are free from fouling.	
	Baffles are correctly installed and oriented.	
Pumps	Suction head meets NPSH requirements.	
Pipes and fittings	Proper gasket installation.	
	Check valve is installed in the correct flow direction.	
	Control valves are operational.	
Instrumentation and Electrical Systems	Control systems are tested and configured.	
	Instruments are calibrated and installed as per layout.	
	Sensors are tested and functional.	
	Emergency shutdown system tested and validated.	
	Grounding and lightning protection verified.	

### 9.1.4 Implementation

After inspecting the plant's operational, mechanical and electrical integrity, the commissioning process progresses to implementing various trials focused on preparing the plant for safe operation before bringing it online. Table 9.2 presents the activities implemented in this phase.

Table 9.2: Commissioning Activities

Activity	Description
Purging and leak testing	The plant's process systems are thoroughly purged using an inert gas to eliminate any residual oxygen or moisture that could create explosive mixtures when flammable gases are introduced. Oxygen concentration within the system is monitored closely to ensure it remains below flammability limits. System leak testing is also carried out with inert gas under pressure to validate containment integrity.
Dry runs and functional testing of control systems	Dry runs are conducted on all rotating machinery including pumps and compressors to resolve any mechanical issues before the introduction of process fluids into the system. Distributed control systems (DCS) are tested for intended response.
Utility system commissioning	All supporting utility systems including steam, cooling water, instrument air, nitrogen supply and power are brought online and tested under load to ensure reliable operation and process stability.
Safety system validation	Involves final testing on fire and gas detection systems, verification of pressure relief devices, flare operation and blowdown systems. Emergency shutdown systems are simulated to ensure rapid and safe shutdowns are achievable under critical conditions.
Performance testing and optimisation	The process units are gradually brought online and monitored. After stable operation is achieved, performance testing is employed to ensure that the plant meets design capacity, yield and efficiency targets. Process parameters are optimised for normal operation and any remaining issues are resolved.

### 9.1.5 Closing Out

The close out phase marks the formal completion of commissioning and transition to full operational status. The plant is handed over to the operation team and this includes the transfer of

documentation, training of personnel and formal approval of stakeholders. At this stage, all plant systems are fully functional and safe for continuous operation. The contractual and performance requirements of the plant would have been met while the operations team is equipped with the confidence to run the plant independently. Nevertheless, ongoing monitoring and maintenance are essential to ensure that the systems perform reliably over an extended period. Any issues that arise should be addressed promptly and documented for future reference.

## 9.2 Start-up Procedure

The start-up phase begins after the successful completion of commissioning and transitions the plant from a pre-operational state to active production. As this process involves the introduction of hazardous chemicals into the system, the objective is to bring the plant to steady state operation at design capacity while minimising any associated risks. The start-up procedure of each process unit on-site is discussed as follows.

### 9.2.1 Reactor Start-up

Table 9.3 outlines the start-up procedure for the epoxidation reactor. During this process, the reactor is initially isolated from the downstream separation units and the reactor effluent is routed to the flare system for safe disposal. The effluent is only directed to the downstream units once the reactor has reached stable operating conditions. This procedure also assumes that the cryogenic distillation unit is already in operation and capable of supplying a steady flow of high-purity oxygen to the reactor.

Table 9.3: Reactor Start-up Procedure

Activity	Description
Reactor purging and warm up	The reactor is purged using dry nitrogen until oxygen levels are well below 1% to prevent explosive mixtures. Purging also removes moisture to prevent catalyst poisoning. Afterwards, the reactor is gradually heated up to its operating temperature to avoid thermal shocks to the catalyst tubes. Operators monitor the reactor's thermal profile to ensure uniform heating and prevent the formation of local hotspots.
Feed Introduction	Ethylene followed by oxygen is fed into the reactor feed line under low flow conditions to ensure that the initial reaction is under control and prevent thermal runaway. Other considerations include maintaining a low oxygen to ethylene ratio to keep the feed mixture outside the flammable range.
Reaction Initiation	The reaction begins once the reactor temperature reaches the catalytic light-off point of 230 °C. Feedback control loops are activated to control the exothermic reaction via adjusting feed composition and increasing coolant flowrate. Operators monitor the reactor outlet gas composition using online gas analysers to keep track of the reaction's progress.
Ramp-up and Stabilisation	As the reactor achieves stable operation, the production rate is gradually increased to the design throughput. Ethylene and oxygen feed rates are slowly increased to achieve steady state conversion. The reactor is ready for operation once the outlet gas composition is within specification.

### 9.2.2 Absorption Unit Start-up

The absorption column is first filled to the required level with water solvent. The solvent recycle pump is then started to initiate solvent circulation through the absorption and flash columns. Once solvent



flow rates are stabilised and system pressures are within operating range, the gas feed valve is gradually opened to introduce reactor effluent into the absorption column. The liquid level in the absorber is continuously monitored and make-up water is adjusted as needed to maintain the setpoint. Simultaneously, the heating system in the flash column is activated and pressure is reduced to initiate flashing. As the system reaches the desired operating conditions, the transfer of rich solvent from the absorber to the flash column is commenced. Startup is considered complete once gas analysers confirm that outlet gas compositions are within specification and steady-state operation is achieved.

### 9.2.3 Purification Unit Start-up

The circulation of hot utility in the reboiler is initiated to gradually heat up the distillation column while cooling medium is introduced into the overhead condenser. Afterwards, the reflux system is activated to establish internal liquid flow. Once the column reaches the desired operating temperature, stripped gas rich in ethylene oxide is gradually introduced. Column operating parameters including reboiler duty, reflux ratio, and pressure are adjusted to achieve the target product purity. Once the product meets specifications, it is directed to storage.

### 9.2.4 Carbon Capture Unit Start-up

The absorber is first filled with potassium carbonate solvent and the solvent circulation pump is started to establish internal flow within the carbon capture system. Once stable recirculation is achieved, the scrubbed gas from the absorption column is directed into the absorber and heat input to the reboiler of the stripping column is gradually adjusted to initiate CO<sub>2</sub> desorption. After the carbon capture unit reaches steady-state operation, the treated reactor effluent gas is routed to the recycle loop for reintroduction into the reactor feed.

## 9.3 Operating under normal conditions

After bringing all process units online, the plant is officially handed over to the operators for normal operation. The plant is defined to be operating under normal conditions if the following criteria in Table 9.4 are met. Under these circumstances, the plant is subjected to achieve an annual ethylene oxide production target of 150 kilo tonnes per annum by operating 8000 hours annually.

Table 9.4: Criteria for Normal Operation

Criteria	Description
Steady-state operation	The plant operates at a constant load with no major fluctuations in production demand.
Reliable equipment performance	No unexpected failure of all process units and ancillary units.
Stable supply chain	No interruption in feedstock availability and logistics network.
No external disruptions	No occurrences of power grid failure, natural disasters or geopolitical issues.

### 9.3.1 Quality Assurance

To ensure product quality during normal operations, the plant's performance is assessed using key performance indicators (KPIs). These KPIs correspond to the design specifications and operational targets of critical process equipment involved in ethylene oxide production. Monitoring these indicators allows operators to verify that the plant is operating within optimal parameters. A summary of the relevant KPIs is presented in Table 9.5 below.

Table 9.5: Key Performance Indicators

Process Equipment	Key Performance Indicators
Epoxidation Reactor R-101	Ethylene conversion of 12.34% Ethylene oxide selectivity of 81.49%
Absorption Column T-101	Ethylene oxide recovery of 99% in absorbent

Flash Column T-104	Ethylene oxide recovery of 99% in vapour phase
Distillation Column T-105	Ethylene oxide product purity of 99.5% by mass

### 9.3.2 Manning Requirements

Daily plant operation requires a well-structured team of skilled personnel to ensure continuous operation. Staffing is structured on a rotating shift basis to provide 24/7 coverage, allowing for continuous monitoring, timely intervention and smooth shift handovers. For plant personnel operations are assumed to follow a three-shift system with each shift lasting 8 hours. Continuous processes conventionally require less personnel due to the plant's high degree of automation. Table 9.6 outlines the key staffing positions and their respective shift arrangements.

Table 9.6: Staff Positions and Shift Arrangements

Role	No. of shifts per day	No. of personnel per shift	Responsibility
Shift supervisor	3	1	Oversee daily operations, ensure compliance with standard operating procedures and facilitate communication between control room and field teams.
Control room operator	3	2	Monitor process parameters, adjust control systems and respond to alarms or deviations in real time.
Field operator	3	10	Conduct routine equipment checks, perform manual interventions and coordinate maintenance activities. Assume 2 operators stationed at each process unit.
Maintenance technician	On-call/ Day shift	4	Handle mechanical, electrical and instrumentation troubleshooting and repairs.
Process Engineer	Day shift only	4	Provide technical support for process troubleshooting and optimisation.
Health, Safety and Environment (HSE) officer	Day shift only	1	Monitor safety compliance and environmental discharges.
Laboratory Technician	Day shift only	2	Conduct product sampling and quality analysis

## 9.4 Shut Down Procedure

A plant shutdown is necessary for inspection and maintenance work to be conducted or in the event of an emergency. The shutdown procedures under both scenarios are discussed as follows.

### 9.4.1 Routine Shutdown

Prior to shut down, the schedule and procedures are communicated clearly across all relevant departments to ensure coordinated execution. Due to the continuous nature of the process, all major process units must be shut down simultaneously. The shutdown begins with a gradual reduction of the reactor feed, ensuring that safe reactant ratios are maintained throughout. Reactor effluent is

diverted to the flare system during this phase. Once feed is fully terminated, the reactor is purged with nitrogen to safely displace residual hydrocarbons and oxygen. Subsequently, feed to downstream separation units is stopped and residual liquids in the columns are drained. These units are then purged with nitrogen to eliminate any remaining volatile compounds. Once all units are safely brought offline, power supplies and mechanical drives are isolated to allow safe access for maintenance. The shutdown concludes with a comprehensive inspection of all process and auxiliary equipment. Checks are performed for leaks, residue buildup and signs of corrosion. Equipment conditions are documented and any maintenance needs are identified and scheduled for resolution during the turnaround period.

### **9.4.2 Emergency Shutdown**

Emergency shutdown procedures are activated in response to critical process deviations or hazardous events that pose an immediate risk to plant personnel, equipment or the environment. Potential triggers include gas leaks, fires, equipment overpressure or failures in control and safety systems. The primary objective is to safely bring the plant to a stable state while minimising potential harm and operational disruption. Emergency shutdowns may be triggered automatically by the Safety Instrumented System (SIS) or manually via emergency stop (E-Stop) stations strategically located throughout the facility. Upon activation, both audible and visual alarms are triggered to alert all personnel. The shutdown sequence begins with the immediate closure of reactor feed valves to isolate the ethylene and oxygen supply. All interconnecting valves between major process units are also closed to halt material transfer across the plant. The reactor is depressurised by routing residual gases to the flare system and vent scrubbers for safe disposal. Simultaneously, downstream separation units are isolated and their liquid contents are drained into designated safe holding systems. Utility systems are shut down in a controlled sequence to terminate heat input while emergency power systems are activated to maintain critical instrumentation, lighting, and control systems. All plant personnel follow the site's emergency evacuation protocol and proceed to designated assembly points. If fires are not extinguished automatically by firefighting systems, trained on-site firefighters are deployed to contain and eliminate the hazard. Once the situation is under control and the area is declared safe, a root cause investigation is initiated. Plant operations are only resumed upon receiving formal clearance from the plant management.

## **9.5 Maintenance**

Effective maintenance strategies are essential to ensure equipment longevity and process safety. A structured maintenance program typically involves a combination of preventative, predictive and corrective maintenance approaches. Since the plant operates for 8000 hours per annum, maintenance activities take place over the 31-day duration of downtime. (Smith, R., & Hawkins, B. (2004))

### **9.5.1 Preventative Maintenance**

Preventive maintenance is a proactive strategy aimed at detecting and resolving potential equipment issues before they lead to failure. By minimising unplanned downtime, it enhances operational reliability and extends the service life of critical plant assets. In the epoxidation reactor, this involves routine inspections of welded seams for corrosion or cracking and continuous leak detection using gas monitoring systems. Downstream separation columns are regularly examined for erosion or damage to internal components such as trays or packing. Rotating equipment including pumps and compressors is subjected to scheduled lubrication and condition monitoring to avoid mechanical breakdowns. Instrumentation and control systems are maintained through periodic calibrations while functional testing ensures the reliability of safety interlocks and emergency shutdown systems.

### **9.5.2 Predictive Maintenance**

Predictive maintenance is a condition-based strategy that relies on real-time monitoring and diagnostic tools to assess equipment health and forecast potential failures before they occur. Unlike preventive maintenance which follows a fixed schedule, predictive maintenance is initiated only when

performance data indicates equipment degradation or an impending fault. This approach minimises unnecessary maintenance and focuses resources where they are truly needed. Vibration analysis is widely used on rotating equipment to detect issues such as bearing wear or misalignment. Thermographic inspections identify abnormal heat patterns in electrical systems, mechanical equipment and heat exchangers to reveal problems like overheating, insulation failure or surface fouling. Ultrasonic testing is employed on pressure vessels and piping to detect internal flaws including corrosion, erosion and cracking. In addition, continuous online monitoring through distributed control systems enables the detection of process anomalies such as pressure or temperature deviations that may signal fouling and leaks.

### 9.5.3 Corrective Maintenance

Corrective maintenance is a reactive maintenance strategy undertaken in response to equipment failure or performance degradation. Its primary goal is to promptly repair or replace faulty components to restore normal operation. This may involve the replacement of a spent catalyst bed in the epoxidation reactor when reduced activity or selectivity is observed which could impact product yield and reactor efficiency. Similarly, packing materials in absorption columns may require replacement if symptoms of fouling or channelling are detected which can compromise mass transfer efficiency and solvent recovery. These interventions are essential to maintaining equipment performance, ensuring process safety and upholding product quality standards.

## 10 Economic Evaluations

This section details the economic evaluation of the designed ethylene oxide plant with a target capacity of 150 kilo tonnes per annum located in Freeport, Texas, USA. The evaluation encompasses the estimation of capital expenditure (CAPEX) and operating expenditure (OPEX), followed by a profitability analysis to determine the economic viability of the project. The design utilises the direct gas-phase epoxidation of ethylene using oxygen over a silver-based catalyst, incorporating cryogenic distillation for on-site oxygen production and a potassium carbonate system with piperazine promoter for CO<sub>2</sub> removal preliminary design study. Therefore, the capital and operational cost of both of site will be calculated.

The economic window examined covers the period from the notice-to-proceed until the fifteenth year of continuous operation. All costs are expressed in US dollars; taxes, depreciation method, discount rate, start-up schedule and working-capital convention are stated explicitly so that every financial metric can be reconstructed. Sensitivity to raw material and utility pricing is explored in a structured parametric study, and finally the investment is judged in terms of profitability and risk relative to typical petrochemical benchmarks.

### 10.1 Capital Cost

The purchase cost of equipment is usually based on the size of the equipment or any other attribute related to the capacity of the equipment. The relation is shown in Equation 10.1

$$C_a = C_b \left( \frac{A_a}{A_b} \right)^n \quad \text{Equation 10.1}$$

Where:  $A$  is the equipment attribute,  $C$  is the purchase cost and  $n$  is the cost exponent. The subscripts  $b$  and  $a$  refer to the base reference equipment and the required equipment attribute respectively.

Most correlations are outdated and require the use of a factor to account for inflation. In this report, the CEPCI is used to calculate the inflation factor. The factor can then be used to find the present purchase cost of equipment,  $C_p^0$ .

The module costing technique introduced by Guthrie (1969) is recommended by Turton (2018) and is cited as being the best for making preliminary estimation of costs. The technique uses the base purchase cost of equipment,  $C_p^0$ , and multiplies its value with factors to account for additional costs. The resulting value is known as the bare module cost,  $C_{BM}^0$  and is the sum of indirect and direct costs of purchasing the equipment. Direct costs include the free on-board purchase equipment cost,  $C_p^0$ , the material required for installation,  $\alpha_M$  and the labor to install the equipment,  $\alpha_L$ . The indirect costs cover the freight, insurance, taxes,  $\alpha_{FIT}$ , construction overhead,  $\alpha_{LO}$ , and contract engineering expenses,  $\alpha_E$ . The equation used to calculate the bare module cost is shown in Equation 10.2

$$C_{BM}^0 = (1.0 + \alpha_M)(1.0 + \alpha_L + \alpha_{FIT} + \alpha_{LO} + \alpha_E) \quad \text{Equation 10.2}$$

$$C_{TM} = C_{BM}^0(1.0 + \alpha_{Com} + \alpha_{Fee}) \quad \text{Equation 10.3}$$

Table 10.1 details the bare module and total module cost for the entire plant. Opportunities for cost saving was kept in mind by specifying when each unit could be made of cheaper materials or designed with a lower design pressure/wall thickness. Cheaper materials such as carbon steel could be used rather than stainless steel when the unit is not in contact with ethylene oxide or any other corrosive material. The factors used for the calculation of these costs are provided in the CAPCOST program (Turton, 2018).

Table 10.1: Capital Cost Summary Table

Compressors	Compressor Type	Power (kilowatts)	# Spares	MOC		Purchased Equipment Cost	Bare Module Cost
C-101	Centrifugal	2660	1	Carbon Steel		\$ 2,230,000	\$ 6,120,000
C-102	Centrifugal	2980	1	Carbon Steel		\$ 2,410,000	\$ 6,590,000

Drives	Drive Type	Power (kilowatts)	# Spares			Purchased Equipment Cost	Bare Module Cost
D-101	Steam Turbine	5000	0			\$ 670,000	\$ 2,340,000

Exchangers	Exchanger Type	Shell Pressure (barg)	Tube Pressure (barg)	MOC	Area (square meters)	Purchased Equipment Cost	Bare Module Cost
E-101	Fixed, Sheet, or U-Tube	4.14	18.5	Stainless Steel / Stainless Steel	857	\$ 391,000	\$ 877,000
E-102	Fixed, Sheet, or U-Tube	3	4.14	Stainless Steel / Stainless Steel	373	\$ 233,000	\$ 525,000
E-103	Fixed, Sheet, or U-Tube	6.72	21	Stainless Steel / Stainless Steel	28.8	\$ 101,000	\$ 223,000
E-104	Double Pipe		6.72	Stainless Steel / Stainless Steel	3.1	\$ 16,200	\$ 35,300
E-105	Fixed, Sheet, or U-Tube	12.5	18.5	Stainless Steel / Carbon Steel	630	\$ 222,000	\$ 556,000
E-106	Fixed, Sheet, or U-Tube	18.5	21	Stainless Steel / Carbon Steel	389	\$ 170,000	\$ 425,000
E-107	Fixed, Sheet, or U-Tube	3	18.5	Stainless Steel / Carbon Steel	605	\$ 208,000	\$ 529,000
E-108	Fixed, Sheet, or U-Tube	4.14	18.5	Stainless Steel / Stainless Steel	91.6	\$ 129,000	\$ 289,000
E-109	Fixed, Sheet, or U-Tube	4.14	21	Stainless Steel / Stainless Steel	994	\$ 433,000	\$ 971,000
E-110	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Carbon Steel	128	\$ 103,000	\$ 257,000
E-111	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Stainless Steel	279	\$ 220,000	\$ 485,000
E-112	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Carbon Steel	857	\$ 278,000	\$ 690,000
E-113	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Carbon Steel	489	\$ 197,000	\$ 489,000
E-114	Fixed, Sheet, or U-Tube	0	25	Stainless Steel / Stainless Steel	1870	\$ 418,000	\$ 1,870,000
E-115	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Carbon Steel	3710	\$ 293,000	\$ 2,910,000
E-116	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Stainless Steel	671	\$ 359,000	\$ 792,000
E-117	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Carbon Steel	197	\$ 124,000	\$ 307,000
E-118	Fixed, Sheet, or U-Tube	25	25	Carbon Steel / Carbon Steel	2120	\$ 136,000	\$ 1,280,000
E-119	Fixed, Sheet, or U-Tube	3	21	Carbon Steel / Carbon Steel	46.4	\$ 38,900	\$ 126,000
E-120	Fixed, Sheet, or U-Tube	3	4.14	Stainless Steel / Carbon Steel	710	\$ 224,000	\$ 575,000
E-121	Fixed, Sheet, or U-Tube	3	3	Carbon Steel / Carbon Steel	272	\$ 72,400	\$ 238,000

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E-122	Fixed, Sheet, or U-Tube	25	25	Stainless Steel / Carbon Steel	164	\$	114,000	\$	284,000	
E-123	Fixed, Sheet, or U-Tube	0	3	Stainless Steel / Stainless Steel	2280	\$	353,000	\$	2,390,000	
E-124	Fixed, Sheet, or U-Tube	3	6.72	Stainless Steel / Stainless Steel	6.1	\$	84,600	\$	191,000	
E-125	Fixed, Sheet, or U-Tube	12.5	21	Carbon Steel / Carbon Steel	46.1	\$	40,700	\$	129,000	
Pump	Type	Power (kilowatts)	# Spares	Discharge Pressure (barg)			Purchased Equipment Cost		Bare Module Cost	
P-101	Centrifugal	13	2	Stainless Steel	21	\$	80,300	\$	158,000	
P-102	Centrifugal	17.5	2	Stainless Steel	3	\$	68,000	\$	148,000	
Reactors	Type	Volume (cubic meters)					Purchased Equipment Cost		Bare Module Cost	
R-101	Jacketed Agitated	550					\$	15,053,000.00	\$	28,965,000.00
Storage Tanks	Tank Type	Volume (cubic meters)					Purchased Equipment Cost		Bare Module Cost	
Tk-101	Floating Roof	5250					\$	724,106.00	\$	796,517.00
Tk-102	Floating Roof	1300					\$	393,565.00	\$	432,935.00
Tk-103	Fixed Roof	3880					\$	389,471.00	\$	428,418.00
Towers	Tower Description	Height (meters)	Diameter (meters)	Tower MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost		Bare Module Cost	
T-101	7.2 meters of 304 Stainless	15.7	3.2	Stainless Steel		25	\$	4,380,000	\$	8,170,000
T-102	5.95 meters of Plastic Saddle	8.59	1.64	Carbon Steel		21	\$	136,000	\$	320,000
T-103	14 meters of 304 Stainless	16	1.35	Carbon Steel		25	\$	227,000	\$	443,000
T-104	54 Stainless Steel Sieve Trays	27	1.66	Stainless Steel		4.1	\$	608,000	\$	1,050,000
Vessels	Orientation	Length/Height (meters)	Diameter (meters)	MOC	Demister MOC	Pressure (barg)	Purchased Equipment Cost		Bare Module Cost	
V-101	Vertical	4.6	2.7	Stainless Steel		2	\$	141,000	\$	359,000
V-102	Vertical	2.68	1.66	Carbon Steel		5	\$	20,600	\$	73,600
V-103	Vertical	1.61	0.54	Carbon Steel		5	\$	4,240	\$	17,300



The grassroots cost refers to the cost of developing a completely new facility on green land. The grassroot cost also account for the outside battery limit (OSBL) costs by adding approximately 20% to 100% of the base case bare module cost (base case refers to the cost of units if using carbon steel as the material of construction). The CAPCOST program uses a value of 50%. Table 10.2 presents all the total module costs and grass roots costs for each unit.

Table 10.2 – Total module, equipment and grass root costs for all units

<b>Total Module Cost</b>	<b>\$87,150,000</b>
<b>Total Grass Roots Cost</b>	<b>\$99,350,000</b>
<b>Total Equipment Cost</b>	<b>\$32,494,082</b>

The chemical plant requires approximately 54,000 m<sup>2</sup> of land which is equivalent to 13.3 acres. Using the price per acre of land close to the desired plant location as a reference. The expected price for the land is \$10,409 per acre (Realtor, 2025). This gives a land cost estimation of \$140,000.

## 10.2 Cost of Manufacture

### 10.2.1 Direct costs

Direct costs are costs that vary with the production volume of the plant. The costs considered in this economic analysis include the raw material, waste treatment, utilities and operating labor.

The cost of raw material is a relatively simple calculation. The dollar price per kg is multiplied by the mass flowrate to determine the annual raw material costs. The feedstocks used in this process include ethylene, methane, water and air. The cost of air is free so is not considered in the summation calculation.

The disposal of waste streams also has a cost as disposing of stream straight into the environment is harmful and unsustainable. The cost of disposal is calculated the same was as the raw material by multiplying the disposal cost per unit mass with the mass flowrate of the waste stream. (S25, S43, S52) Table 10.3 summarises the calculations of raw material and waste disposal costs.

Table 10.3 – Raw material and waste disposal costs

<b>Material Name</b>	<b>Classification</b>	<b>Price (\$/kg)</b>	<b>Flowrate (kg/h)</b>	<b>Annual Cost</b>
Ethylene	Raw Material	\$0.69	17057.80	\$97,948,958
Methane	Raw Material	\$0.15	2720.20	\$3,395,626
Ethylene Oxide	Product	\$1.39	17894.00	\$206,990,277
Purge stream	Non-Hazardous Waste	\$0.01	3904.00	\$454,847
Heavy waste	Non-Hazardous Waste	\$0.01	137317.00	\$15,998,529
water	Raw Material	\$0.0006	649198.00	\$3,241,575

Utilities as calculated in a similar way to the raw material, the only difference is that a unit of energy is used instead of mass. Due to the heat integration technique employed, there is no hot utility requirement. All the utilities costs come from the use of cold utilities include refrigeration and process water. The utility costs for each process unit is provided in Table 10.4

The cost operating labour is estimated using the simplified correlation developed by Alkhayat and Gerrard (1984) in Equation 10.4.

$$N_{OL} = (6.29 + 0.23 N_{np})^{0.5} \quad \text{Equation 10.4}$$

Where  $N_{OL}$  is the number of operators required per shift and  $N_{np}$  is the number units including compressors, towers, reactors, heat exchangers.

For this process the number of operators can be calculated as 3.9 operators per shift. Turton (2018) recommends hiring 4.5 operators per operator required to ensure availability for all shifts (3 per day). This leads to an estimated 18 operators to be hired for the plant.

Assuming an operator works 49 weeks a year and 40 hours a week, an operator will work approximately 1960 hours in a year. The hourly salary in Texas for an operator is \$32.02 (Indeed, 2025). This gives an estimated salary of \$66,910 per year and total \$1,137,470 per year on labor costs.

### Fixed costs

Fixed costs represent the annual expenditures that the ethylene-oxide facility must bear simply to exist and remain in operable condition; by definition they are insensitive to how many tonnes of product leave the battery limit each year. They include property taxes, insurance, depreciation and plant overhead costs.

Plant depreciation according USA federal tax law is operated on MACRS (Modified Accelerated Cost Recovery System) (Turton (2018)). MACRS operating over a selected class life for the case of chemical equipment with no salvage value depreciates using either a double declining balance method or a straight line method in accordance with whichever one gives a higher rate of depreciation allowance for that half year. The depreciation counts as a tax deductible, so having a higher depreciation value gives a higher NPV of funds recuperated.

### Working Capital

The working capital,  $C_W$ , is the sum of money required to fund the operating costs at the start of the plant life. Turton (2018) provides Equation 10.5 to estimate the working capital cost.

$$C_W = A \times C_{RM} + B \times FCI_L + C \times C_{OL} \quad \text{Equation 10.5}$$

### Total Cost of Manufacture

The total cost of manufacturing,  $COM$ , is given in Equation 10.6

$$COM = 0.18 \times FCI + 2.73 \times C_{OL} + 1.23(C_{UT} + C_{WT} + C_{RM}) \quad \text{Equation 10.6}$$

## 10.3 Profitability Analysis

This section uses the standard discounted cash flow framework to demonstrate whether the ethylene oxide project creates value over its 15-year economic life.

The evaluation begins with the discounted cash-flow (DCF) diagram, reproduced in Figure 10.1. The horizontal axis records time in fiscal years from the final-investment-decision date, while the vertical axis shows cumulative net cash after discounting at the rate of 10%. Figure 10.1 also illustrates the chosen capital distribution, sixty per cent of the total investment is disbursed in Year 1 (to cover long-lead equipment, detailed engineering and site civil works) and the remaining forty per cent is paid in Year 2 as mechanical completion approaches.

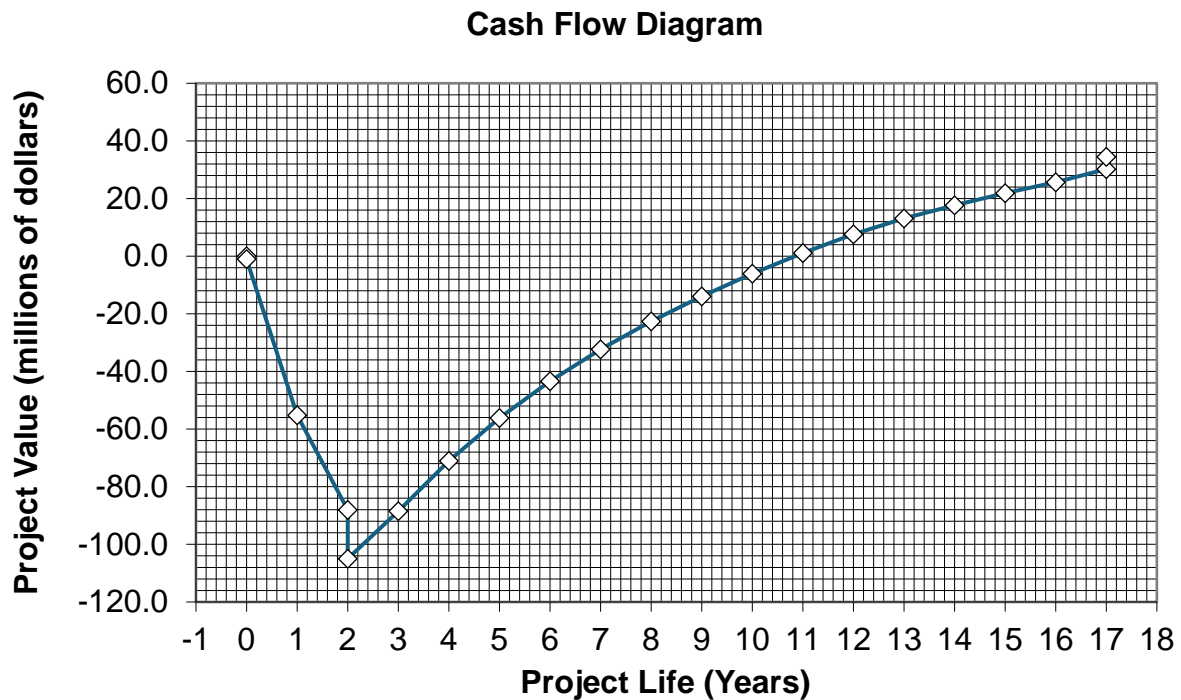


Figure 10.1 – Discounted cash flow diagram of project

The discounted pay-back period identifies the calendar year in which cumulative, discounted cash flow first becomes positive. In the present cash curve, the initial capital of \$99,350,000 is recouped in 6.5 full years of operation. The discounted pay-back period accounts for the time value of money and all cash flows after crossover.

The discounted cash flow rate of return (DCFROR) is defined as the discount rate that makes the net present value (NPV) of a project zero. The NPV is the difference between the present value of cash inflows and the present value of cash outflows. For this plant, the DCFROR calculates to 15.0%, and the NPV is calculated as \$34.47M

The plant assets are depreciated using the MACRS over a 10-year period. Depreciation itself is non-cash, yet it shields taxable income and therefore influences every profitability metric above. Together, the discounted cash-flow diagram, pay-back period and DCFROR provide a coherent picture of economic viability of the plant.

## 10.4 Parametric/Uncertainty Analysis

To evaluate the economic risk under varying market conditions, product and reactant prices are varied using the uncertainty of them changing in a Monte Carlo simulation. Upper and lower limits of variances of variables are established in advance for this analysis with the bounds be stated in Table 10.4 below

Table 10.4: Monte Carlo variable ranges

<u>Variable</u>	<u>Lower Limit</u>	<u>Upper Limit</u>	<u>Base Value</u>
FCIL	-20%	30%	\$99,350,000
Price of Product	-10%	5%	\$206,990,277
Working Capital	0%	0%	\$20,500,000
Income Tax Rate*	0%	0%	45%
Interest Rate*	0%	0%	10%
Raw Material Price	-10%	10%	\$104,586,159

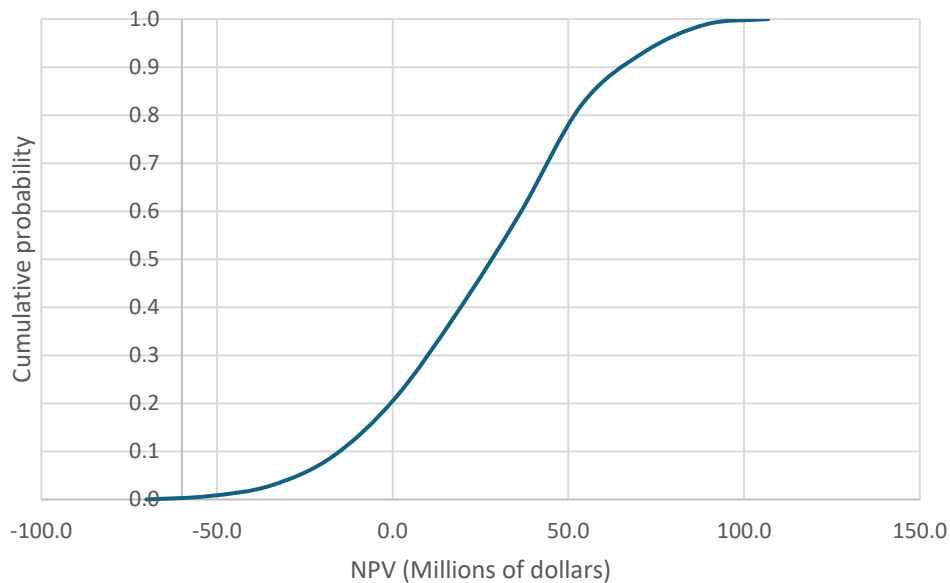


Figure 10.2: NPV against cumulative probability

With the Y axis representing the cumulative probability and the X axis representing the NPV in millions of dollars, Figure 10.2 shows that there is only a 10% chance that variable market conditions might lead to a diminished Net Present Value whereas a growth in NPV of 50 million dollars is rated at a 20% likelihood. It should be noted that these percent likelihoods reflect expected nominal market fluctuations and not particular active political factors that may affect the market. The takeaway from this figure is that it is highly unlikely that market will drop enough as to render this plant unprofitable.

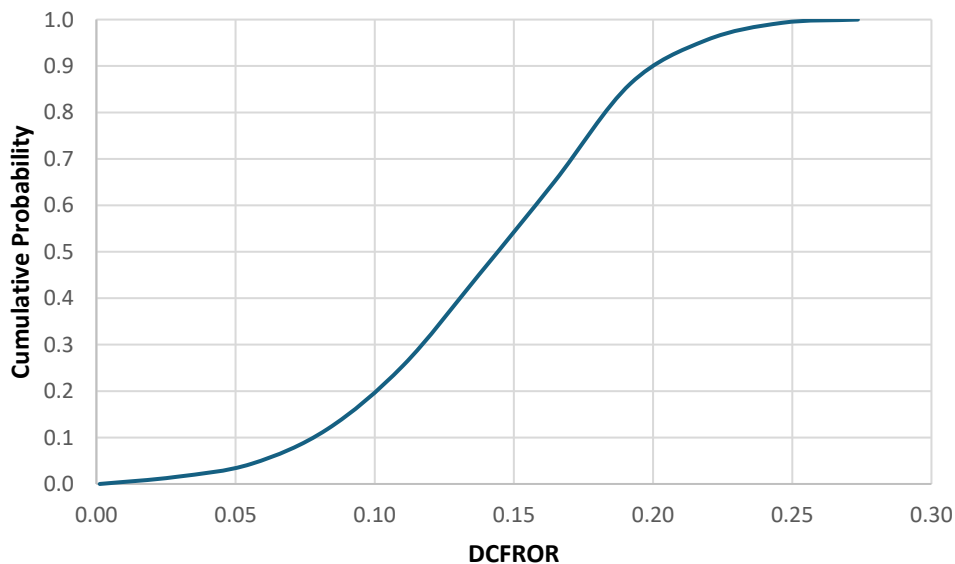


Figure 10.3: DCFROR against cumulative probability

Figure 10.3 shows that will the discounted rate of return is somewhat uncertain only claiming a 60% chance that it will not change by more than 5%, the chances of the rate of return diminishing beneath 5% are less than 5%.

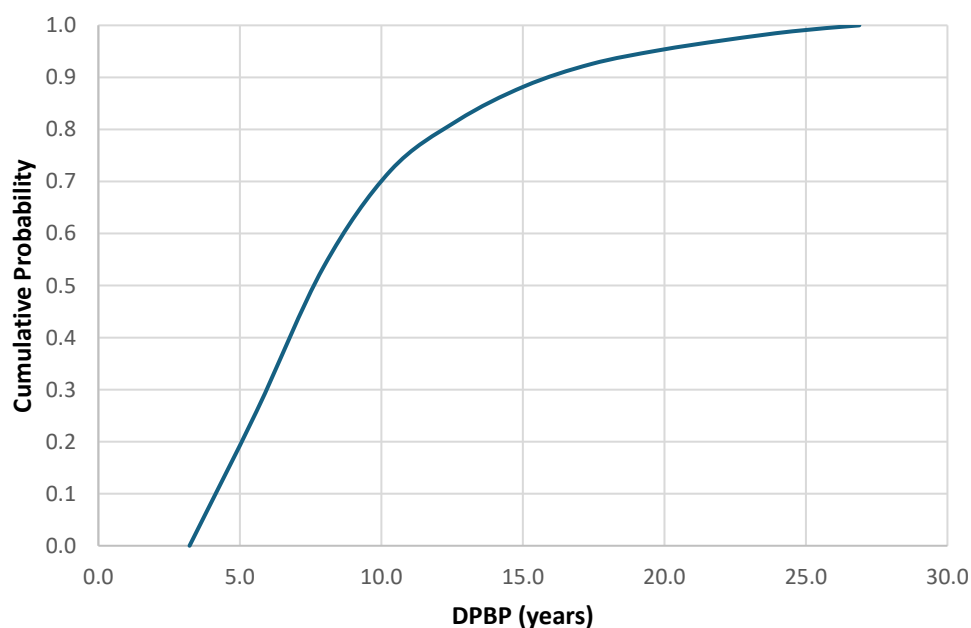


Figure 10.4: DPBP against cumulative probability

Figure 10.4 graphs the discounted payback period against the probability the sum will have been paid back in that many years. While there is very little room for the investment to be paid back significantly earlier than expected, there is an 88% chance that the plant will be paid back within its operation lifespan after accounting for the time value of money and inflation. There is also a 70% probability that the plant will be paid back within 10 years of the start of construction when considering the variables in table 10.4.

## 11.0 Conclusion

### 11.1: Summary of Work

This report finalises the plant design for the sustainable production of ethylene oxide, finding the plant design to be profitable. The plant was optimised around the reactor and recycle loop to reach the minimum Partial Annualised Cost while still generating the design 150 kilo tonnes per annum after distilling to 99.5% purity. Reducing the operating expenses by 3 million dollars per annum, the optimised parameters gave: purge fraction of 1.07%; reactor length of 14.4 m; reactor inlet pressure of 18.5 bara; 168.9 mol/s of ethylene feed; 157 mol/s of oxygen feed; 47.1 mol/s of methane. These mark a reduction in feed flowrates, reducing the amount of reactant wasted in the purge. These adapted flowrates were used to generate a comprehensive Mass and Energy balance. Conducting the heat integration across this process finds that the heating requirements can be entirely satisfied by process to process heat transfer, removing the need for hot utility generation under standard operation.

Changes to the plant design since part 1 were incorporated into the plant PFD and P&ID with the largest change being removing what was previously distillation column T-105. The plant layout taking up a 258 m by 194 m plot in an industrial park in Freeport, Texas, has subsections for the process unit plot, tank farm, boiler house and ancillary buildings. Plant safety is considered in the plant layout with 30 m gap between process plot, tank farm and boiler house as well as the carpark and most

of the ancillary buildings being are the far side of the plant from the flammable chemicals. The boiler house containing the flare and the reactor R-101 are both kept distant from the ethylene, methane and Ethylene Oxide tanks, ensuring that in the event of a process thermally rupturing, the stored chemicals are not liable to cause a larger explosion. The onsite oxygen distillation and water treatment facilities as well as CHP unit reduce the plants dependence on market availability of water, electricity and oxygen. On site power generation is of particular value as it isolates the plant from major power outages such as the power grid failure for Texas in 2021.

The plant is expected to cost 99.35 million dollar to build, with a yearly profit of 32 million dollars, generating an expected payback time of 6.5 years and a total adjusted profit across the plant life of 15 years. The return on investment is 15% making the plant highly lucrative.

For the plant to be considered sustainable, the environmental and social pillars must be supported beyond the profitability assessment. With dedicated carbon capture columns for the recycle, heat integration greatly decreasing the process's operating carbon footprint as evaluated from conducting a LCA, and using vent gases in a CHP unit to reduce grid reliance, the finalised design operates with minimal emissions without compromising profitability. This works out to a global warming potential of 432900 tonnes of CO<sub>2</sub> equivalent emissions per annum of which 67% of the contribution is from the sourcing of raw materials.

## 11.2 Reflection on Accuracy

When conducting this project key assumptions of: no by-product formation of Ethylene Glycol or organic acids formed from ethylene; downstream units continue to perform similarly during the optimisation; that the environmental burdens associated with grid power and sourcing reactants remain similar to those represented in the CCalc2 database from 2007-2010, and that recent political developments in the USA do not render sourcing the reactants or selling the product to China infeasible. The assumption of no significant byproducts being formed is controlled through reactor conditions and materials being unfavourable to undesired reactions. The impact of the outdated database for the LCA while significant, is reduced by the site's independence from the state power grid and from oxygen suppliers and water suppliers.

## 11.3: Reflection on Development

As a months long project, this coursework requires the team to bring together their studies into a cohesive whole, gain experience about working in a group over long timespans and manage project timelines. The project required developed planning and initiative requiring the team to figure out what process units would be required for the process and reevaluating the necessity of each unit across the progression of the design. This was particularly relevant for restructuring the design after the changes made in part 2, requiring clear communication about changes made as the project is too broad to be conducted without subdivision.

Evaluating the viability of the plant at large encourages thinking about the process at a whole when designing any of the individual systems. The economic viability assessment forces the team to consider that even after all the efforts put in to find an optimise a design, putting a given design into practice is not necessarily profitable.

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