UNIVERSITY of
HOUSTON
CULLEN COLLEGE OF ENGINEERING
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Chemical and Biomolecular Engineering

Ethylene Glycol Plant

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Letter of Transmittal

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Dear Dr. Fleischer,

We, the undersigned students, submit our midterm report titled ‘Senior Design Project'. The report explains the methodology of designing and the calculations for material balances, energy balances, and cost analysis. The proposal includes a detailed PFD and also discusses the simplifying assumptions made for calculations, followed by an in-depth discussion on the results and recommendations to improve the design. The report also includes environmental and safety analysis, including the flammability diagrams.

All four team members contributed to the development of the project. Although each team member had the responsibility of their respective unit operations, however, for important decisions there were discussions to reach an agreement. This collaborative effort resulted in the successful completion of the project.

Below is the breakdown of the tasks that each team member was responsible for:

Sehar Allana was responsible for the designing and material and energy balance calculations of the EO Scrubber, EO Desorber, CO2 Scrubber, and some Heat Exchangers. She also helped Huong with the recycle loop for Reactor 1. Sehar then worked on the sizing and the cost analysis for the EO Scrubber, EO Desorber, CO2 Scrubber, mixers and splitters, and all the pumps and compiled the cost estimation sheet for the plant.

Gage Attard worked on designing and doing preliminary mass balances for Reactor 1 and the energy balances on the compressor and the pumps. He was responsible for drawing out all the equipment and writing out the stream data for the PFD. Gage also worked on the chemical compatibility for all the equipment to see what would be the best construction material and was responsible for the sizing and cost analysis for all the Heat Exchangers.

Benjamin Perez designed the Ethylene Glycol recovery section of the plant, comprising of Evaporator 1, Evaporator 2, MEG Column and the relating Heat Exchangers, Pumps and Valves. He performed the mass and energy balances for these above-mentioned unit operations, followed by the sizing and cost analysis on the Evaporator 1, Evaporator 2, and MEG Column and the valves. He also compiled the raw materials & utility costs for the plant.

Huong Phan developed the mass and energy balances for Reactor 1, Reactor 2, and worked on Reactor 1 recycle loop with Sehar. Huong also took the lead in performing the flammability calculations and developing the flammability diagrams. Furthermore, she did the sizing and cost analysis on Reactor 1 and 2.

We thank you for all your input and advice on the preliminary designs and hope that this report satisfies all the project requirements.

Below are the signatures of all the members, acknowledging that to the best of our knowledge all the presented information is correct, and no commercial stimulator was used for Phase 1 of the Project.

Thank you,

Sehar Allana
Ben Perez
Gage Attard
Huong Phan

Abstract

The purpose of this project was to design a model that can reach the production requirement of 700 kTA of ethylene glycol in the most effective way. The project is divided into five sections: ethylene epoxidation reactor, separation of ethylene oxide, CO2 capture for ethylene recovery, non-catalyst hydrolysis of ethylene oxide, and separation of ethylene glycol products.

The current design produces 708 kTA of mono ethylene glycol (MEG) with 99.9% purity and a total capital investment of $241,619,000. The report analyzes the methods and equations used in designing the PFD, cost, and safety analysis and details the mass and energy balances.

Ethylene glycol is an odorless, colorless, sweet-tasting, viscous liquid that can be made by the reaction of ethylene oxide with water, where ethylene oxide is an important, ethylene-based intermediary compound.

Ethylene oxide is a product of ethylene and oxygen reacting over a silver catalyst surface. Partial oxidation of ethylene goes to ethylene oxide and, the rest goes to carbon dioxide and water. The major cost in the production of ethylene oxide is ethylene, hence, it is important to optimize the selectivity towards ethylene oxide and thus reduce the consumption of ethylene. The proposed plant has the selectivity set to 10% with a recycle loop to increase the efficiency use the unreacted reactants.

In the production of ethylene glycol, one mole of ethylene oxide reacts with 21 moles of water in a liquid phase tubular reactor with a 100% conversion. Three reactions occur in total where the most reacted ethylene oxide goes to ethylene glycol and, a small amount goes to the byproducts which, mainly include di-ethylene glycol (DEG) and tri-ethylene glycol (TEG).

Assumptions were made based on the study of the literature throughout the process. Multiple studies on thermodynamic, unit operations and chemical processes have also been done to prepare for this project.

Some of the challenges included purging the inert from the recycle loop for Reactor 1 and the recovery of ethylene glycol, particularly in choosing the right unit operations and performing mass balances.

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1. Introduction

1.1. Background

Ethylene glycol serves many purposes in various industries. For instance, it is used as an engine coolant and a precursor for polymers which are used in the production of various items we use every day such as polyester clothes, plastic bottles, etc. Because of this, it is paramount to properly and efficiently produce this compound. The market for ethylene glycol products is expected to reach $47.26 billion by 2025, with mono-ethylene glycol (MEG) encompassing 89.9% of the current total market share. In addition to this, the market share of MEG is growing at a faster rate than the other ethylene glycols as the beverage market is expanding and requiring more MEG to manufacture polyethylene terephthalate (PET) plastic. In 2018 the rapidly growing Asia Pacific market accounted for approximately 44% of this demand, which indicates that the forecasts of increased demand are likely accurate, and there will be continuous growth in the ethylene glycol market.

Ethylene glycol was first produced in 1856 by French Chemist Charles-Adolphe Wurtz. The mechanism of production was treating ethylene iodide with silver acetate to create ethylene diacetate. The ethylene diacetate was then hydrolyzed with potassium hydroxide to yield ethylene glycol. The resulting compound was named glycol, as its shared qualities of both ethyl alcohol and glycerin. Wurtz then created the same compound via ethylene oxide in 1859, but it still was not commercially produced at this time.

Semi-commercial manufacture of ethylene glycol began around WWI as a substitute for glycerol in explosives manufacturing. In 1917 Carbide and Carbon Chemical Company launched the first large-scale plant in the United States and produced essentially all ethylene glycol manufactured in the US via ethylene chlorohydrin. This method is done by reacting ethylene and chlorine in water, concentrating that solution, and hydrolyzing it to ethylene glycol with sodium bicarbonate in a closed, steam jacketed vessel. The issue with this method is that it is slower and more difficult to separate the MEG from other salt byproducts.

In 1937 Carbide and Carbon Chemical Company began to use vapor phase EO production as the first step in the ethylene glycol production process, which is used today. Carbide and Carbon Company maintained control of this direct oxidation process in the US until the 1950's when the process was offered for licensing and commercialization.

1.2. Project

We are a team of chemical engineering seniors at the University of Houston, and our goal is to design a process for producing 700 kTa of MEG. The feedstocks we are provided are ethylene, oxygen, and water. We are completing this project-based on-site data for a chemical processing facility in the US Gulf Coastal Region. The method of production we are focused on is what is currently industry-standard - the production of MEG through first oxidizing ethylene to ethylene oxide (EO) over a silver catalyst, then hydrolyzing the EO to MEG, DEG, and TEG. Our target for this project is a 99.9% pure MEG stream.

We are doing this project to demonstrate our understanding of the concepts, theories, and techniques we have learned throughout our curriculum. For this semester, we will avoid using commercial process simulators and rely on our knowledge to accomplish this task.

Ethylene glycol is produced today commercially almost exclusively by the hydrolyzation of ethylene oxide. Ethylene oxide is a highly reactive chemical primarily produced by the catalytic oxidation of ethylene. The reaction between ethylene and oxygen occurs under a temperature of approximately 230^oC and a pressure of approximately 20 bar. The important reactions that occur are:

$$Ethylene\ + \frac{1}{2}\ O_2\ \rightarrow\ \ Ethylene\ Oxide \text{ (Desired)}$$

$$Ethylene + 3\ O_2\ \rightarrow\ 2CO_2 + 2H_2O \text{ (Undesired)}$$

$$Ethylene\ Oxide + \frac{5}{2} O_2 \rightarrow 2CO_2 + 2H_2O \text{ (Undesired)}$$

The per-pass ethylene conversion is limited from 8% to 10% to minimize the side reactions (reactions 2 and 3). At higher ethylene conversion, the ethylene oxide concentration lies within the flammability envelope [4]. For safety purposes, methane was added to saturate the system and reduce the risk of explosion at the reactor inlet [27]. This reduces the chance of an explosion through the practice of engineering controls. From here ethylene oxide is removed from the reactor outlet vapor stream and separated from unreacted components and side products. This separation is done by a series of scrubbing, stripping, and distillation columns. After the separation, the EO is mixed with water and sent downstream to the ethylene glycol reactor. The reaction between ethylene oxide and water in a non-catalytic tubular reactor occurs under a range of temperature and pressure at 180-230^oC and 200-370 psia, respectively. In 2018, 73% of the ethylene oxide market was consumed to produce mono-ethylene glycol, di-ethylene glycol, tri-ethylene glycol, and a small number of heavier glycols [3], with MEG, accounts for approximately

90% of the market for ethylene glycol. The three main reactions that we are focusing on are:

$$Ethylene\ Oxide + H_2O \rightarrow Ethylene\ Glycol \text{ (Desired)}$$

$$Ethylene\ Oxide + Ethylene\ Glycol \rightarrow Diethylene\ Glycol \text{ (Undesired)}$$

$$Ethylene\ Oxide + Diethylene\ Glycol \rightarrow Triethylene\ Glycol \text{ (Undesired)}$$

The yield of MEG via hydrolysis is controlled by the water-to-ethylene oxide ratio in the feed to the reactor system. The more water we feed in the system the higher selectivity of MEG to ethylene oxide that reacts. In practice, reactor feed water content is such that the selectivity to MEG achieved ranges from 89-91%, because the more water we feed in, the more unreacted amount of water that needs to be removed, and it requires capital investment in evaporators [19]. The evaporation system can be modeled as a series of distillation towers, with water being the light key (LK) The ethylene glycol reactor outlet stream is sent to our flash system where water is flashed into the vapor phase and recycled back to the reactor, while the glycol products are sent downstream to product separation. After MEG, DEG, and TEG are produced in the reactor and the water is removed, the glycol products are sent to a series of product distillation columns. In a typical chemical processing facility MEG, DEG, and TEG would all be separated into 99.9% pure streams and sold to maximize profit, but for this project, we are only concerned with separating the MEG stream. To accomplish this, we require only a single distillation column where we will have a distillate stream of 99.9% pure MEG, and a bottoms stream of primarily DEG and some TEG.

In the end, to summarize the project specifications, refer to the following tables:

Table 1- Unit Design Target

Production rate of EG	700 kTA
On-Stream factor	8400 hrs/yr

Table 2 - Design Feedstocks Properties

Component	Composition (wt%)
Ethylene	99.9
Ethane	0.1
Total	100

Component	Composition (wt%)
Oxygen	99.8
Argon	0.2
Total	100

Table 3 - Product Specifications

Product	Composition (wt%)
EG	99.9
DEG	0.05
Water	0.05

2. Methodology

2.1. Ethylene Epoxidation Reactor

2.1.1. Assumptions

The material balances were calculated based on a given ethylene oxide selectivity of 0.85. Assuming only 10% of the feed-in ethylene will react with O_2 per pass and only 85% of reacted ethylene will go to ethylene oxide and 15% will go to produce CO_2 and water. The required amount of feed-in oxygen is first calculated based on the ratio of the three reactions. A half mole of O_2 is needed to produce 1 mole of ethylene oxide, and by assuming both reaction 2 and 3 will need 3 moles of O_2 (reaction 3 needs 2.5) to produce 2 moles of CO_2 and 2 moles of water, we can get the total mole of O_2 needed per-pass. Based on the research on commercial plants, the amount of feed-in O_2 is about 1/3 of ethylene. If reaction 3 is dominated, the only difference is we will have a small extra amount of unreacted O_2 that needs to be recycled because the reactor will still produce the same amount of CO_2 and water. The temperature throughout the reactor is maintained at 446^{o}F under steady operation.

2.1.2. Material Balance

For: Ethylene = A
Oxygen = B
Ethylene Oxide = C
Carbon Dioxide = D

Water = E

All of the values were found by applied equations below. Based on the given selectivity, S, with the feed-in ethylene molar flow rate at 10% conversion, we can calculate the amount of ethylene oxide produced per pass.

$$S = \frac{mole\ of\ ethylene\ oxide\ produced}{mole\ of\ ethylene\ reacted} = 0.85$$

$F_{A\_reacted} = F_{Ao} * 0.1$

$F_C = F_{A\_reacted} * 0.85$

The rest of the reactant ethylene goes to make CO_2 and water with the ratio of 1 mole of ethylene produced 2 moles of CO_2 and 2 moles of water. Then, we have:

$F_D = F_{A\_reacted} * (1-0.85) * 2$

$F_E = F_D$

After all of the production values are found, we can use it to back-calculate the total mole of O_2 that reacted.

For reaction 1: $F_{B1\_reacted} = 1/2 * F_C$

For reaction 2 + 3: $F_{B2\_reacted} = 3/2 * F_D$

Total: $F_{B\_reacted} = F_{B1} + F_{B2}$

The amount of unreacted ethylene and oxygen can be found by subtracting the reacted values from their initial values. As stated earlier, the amount of feed-in O_2 is about 1/3 of ethylene.

$F_A = F_{Ao} - F_{A\_reacted}$

$F_B = F_{Bo} - F_{B\_reacted} = (1/3) * F_{Ao} - F_{B\_reacted}$

2.1.3. Energy Balance

For energy balance calculation, reaction 3 occurred when 1 mole of ethylene produced 1 mole of ethylene oxide and the product continues to react with O_2 to produce CO_2 and water. However, reactions 2 and 3 produce the same amount of CO_2 and water, we can combine both reactions and assume that the change in enthalpy for both reactions is based only on ethylene, CO_2, and water. Since selectivity was the only provided information, the calculation will only focus on the inlet and outlet of the reactor.

We started the calculation with the general energy balance equation [18].

$$\dot{Q} - \dot{W} + \sum_{i=1}^{n} F_{io} H_{io} - \sum_{i=1}^{n} F_i H_i = \frac{d\hat{E}_{sys}}{dt}$$

After making these assumptions: steady-state, no phase change, and no work, the energy balance equation becomes [18].

$$\dot{Q} - F_{Ao} \sum \theta_i C_{Pi}(T - T_{io}) - \Delta H_{Rx}(T) F_{Ao} X = 0$$

The reactants will be entering the system at the same temperature, so:

$$T = T_{io}$$

The equation becomes:

$$\dot{Q} - \Delta H_{Rx}(T) F_{Ao} X = 0$$

And for our reactions, the equation rearranged to:

$$\dot{Q} = \Delta H_{Rx1} F_{Ao} X_{A1} + \Delta H_{Rx2} F_{Ao} X_{A2} + \Delta H_{Rx3} F_C X_C$$

For reaction 3 to happen, we needed 1 mole of ethylene to produce 1 mole of ethylene oxide, and reactions 2 and 3 are produced the same amount of CO_2 and water, we can combine both reactions and assume that the heat of reactions are the same for both, at the outlet of the reactor we have:

$$\Delta H_{Rx2} = \Delta H_{Rx3}$$

$$\dot{Q} = \Delta H_{Rx1} F_{Ao} X_{A1} + \Delta H_{Rx2}(F_{Ao} X_{A2} + F_C X_C)$$

$$F_{Ao} X_{A1} = F_{A\_reacted} * 0.85$$

$$F_{Ao} X_{A2} + F_C X_C = F_{A\_reacted} * (1-0.85)$$

$$\Delta H_{Rx1} = H_C^o - \left(\frac{1}{2}\right) H_B^o - H_A^o + \left[\left(C_{PC} - \left(\frac{1}{2}\right) C_{PB} - C_{PA}\right) * (T - T_R)\right]$$

$$\Delta H_{Rx2} = 2H_D^o + 2H_E^o - 3H_B^o - H_A^o + [(2C_{PD} + 2C_{PE} - 3C_{PB} - C_{PA}) * (T - T_R)]$$

$T_R = 76.73^oF$

All of the H_i^o and C_{Pi} values are found based on the Thermodynamic textbook [16], and the total energy that needed to be removed from the reactor can be calculated.

2.2. Separation of Ethylene Oxide & CO_2 Capture for Ethylene Recovery

2.2.1. Assumptions

For the absorber and stripper calculations, a graphical method for the trayed tower was used [30]. A phase equilibrium is assumed between the vapor and the liquid leaving each tray. It is also assumed that the only solute is transferred from one phase to the other and the temperature is constant hence, K (equilibrium constant) is constant throughout the tower.

Kremser Chart (Appendix 1) was used to approximate A and S, absorbing factor and stripping factor, respectively. This was based on the number of trays for each column.

$$y_i P = x_i H$$

Henry's Law, the equation above, was used to assume a plausible mass composition of the components other than the solute and absorbent.

To determine the composition of the other components in stream 54 some assumptions had to be made through research. For this design, ethane, argon, and methane are inert hence it is assumed that their solubility is negligible in the amine solution. Oxygen has a decreasing solubility with "with increasing carbon dioxide loading of the amine" so it can be assumed that the oxygen solubility is negligible hence the solubility of oxygen was very small [13].

For ethylene and ethylene oxide it is assumed that less than 1% of the EO Scrubber feed is dissolved in the amine solution with carbon dioxide. The reason this assumption is made is that we know that hydrocarbons are soluble in amines so with the given data and research it is reasonable to make the above-mentioned assumption [30].

2.2.2. Material balance

$$V'^{Y_{N+1}} + L'^{X_0} = V'^{Y_1} + L'^{X_N}$$

$$V_{N+1} + L_0 = V_1 + L_N$$

- Absorber (EO Scrubber & CO_2 Scrubber)

        - $Y_{N+1}$and X_0were calculated using equations above, respectively.
        - A number of stages were selected.
        - L' was calculated using the L'/V' ratio.
        - K was calculated using Appendix 1.
        - An initial value for Y_1 is assumed for trial and error.
        - Excel Solver was used for trial and error.
            - Number of stages and Y_1 were the changing parameters for the EO Scrubber and the CO_2 Scrubber, L'/V' was also a changing parameter.
            - Solver was run a couple of times until the optimum number of stages and Solute recovery was achieved.
                - EO Scrubber: 21 stages with about 99% recovery.
                - CO_2 Scrubber: 9 stages with 93% CO_2 recovery and a ratio of 1.99 which is plausible.
    - Stripper (EO Desorber)
        - $Y_{N+1}$and X_0were calculated using Equations listed above, respectively.
        - A number of stages were selected.
        - V' was calculated using V'/L'.
        - K was calculated using Appendix I.
        - An initial value for Y_1 is assumed for trial and error.
        - Excel Solver was used for trial and error.
            - Number of stages and Y_1 were the changing parameters.
            - Solver was run a couple of times until the optimum number of stages and EO recovery was achieved which in our case was 21 stages with about 99% recovery.

2.2.3. Energy balance

$$Q = \Delta H$$

Since there is no change in the temperatures within the phase, $\Delta H = 0$, hence Q = 0. EO Scrubber, EO Desorber, and CO_2 Scrubber are all adiabatic units.

2.3. Non-Catalytic Hydrolysis of Ethylene Oxide

2.3.1. Assumptions

An assumption of 99.99% conversion of ethylene oxide was made based on ethylene oxide's high reactivity.

2.3.2. Material Balance

We calculated the possible percent of MEG might lose during the separation to get the pure substance, then we added the possible loss to the requirement and got the total amount of MEG that we need to produce per cycle. The amount of water feed in the reactor is 21 to 1 mole of the feed-in ethylene oxide. The rates of all three reactions were calculated based on the given pre-exponential and activation energy, see Table 4. The reactor effluent stream contains the new production of MEG, DEG, TEG, and a huge amount of unreacted water. The amount of unreacted water will then separate and be sent to wastewater treatment, and the desired, undesired products will be sent for further separation.

For: Ethylene oxide = A
Water = B
MEG = C
DEG = D
TEG = E

All of the values in Table 4 were found by applied equations below. The design general mole balance equation for PFR in molar flow rate and concentration is [17]:

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

$$\frac{dF_B}{dV} = r_B$$

$$\frac{dF_c}{dV} = r_c$$

$$\frac{dF_D}{dV} = r_D$$

$$\frac{dF_E}{dV} = r_E$$

$$r_A = -k_1 C_A C_B - k_2 C_A C_C - k_3 C_A C_D$$

$$r_B = -k_1 C_A C_B$$

$$r_C = k_1 C_A C_B - k_2 C_A C_C$$

$$r_D = k_2 C_A C_C - k_3 C_A C_D$$

$$r_E = k_3 C_A C_D$$

Find k by using the Arrhenius equation with the chosen operating temperature (431^{o}F) and the given pre-exponential, activation energy in Table 3.

$$k = A * exp\left[-\frac{E_A}{RT}\right]$$

Table 4 - Pre-exponential and activation energy values

Reaction	An (m^3/Kmol-s)	E_A (KJ/Kmol)
1	5.3×10^5	78000
2	1×10^6	82000
3	2×10^6	81000

Because all of the reaction rates have concentration terms in them, we will use the general mole balance in concentration form for calculation.
The feed flow rate of ethylene oxide, F_{Ao}, is given, and F_{Bo} is calculated based on the assumption of ethylene oxide – water ratio.
15 moles of water to 1 mole of ethylene oxide, we have:

$F_{Bo} = 15 * F_{Ao}$

Assumed the amount of feed-in ethylene oxide is small compared to water and the density of water stays constant, we can find the total volumetric flow rate:

Mass flow rate of water (lb/hr) = $F_{Bo} * MW_B$

ρ_B = density of water = 62.4 (lb/ft^3)

MW_B = molecular weight of water = 18 (lb/lbmol)

$$v_o = \frac{mass\ flow\ rate\ of\ water}{\rho_B}$$

The concentration of all components at its initial state is found by using v_o:

$C_{Ao} = F_{Ao} / v_o$

$C_{Bo} = F_{Bo} / v_o$

With all of the information above, by using an Excel spreadsheet, we can find the reactor outlet flow rates for all components at any given volume.
We started the Excel calculation with no recycle stream assumption, so we only have ethylene oxide and water are fed to the reactor. The other component initial concentrations are:

$C_{Co} = C_{Do} = C_{Eo} = 0$

Next, the Euler method will be used to show the changing of each component concentration over the changing of reactor volume. From the general mole balance equation, we have:

$$C_{A(n+1)} = \frac{r_{An}}{v_o} * dV + C_{An} \qquad \text{for n = 0,1,2…}$$

With: $r_{An} = -k_1 C_{An} C_{Bn} - k_2 C_{An} C_{Cn} - k_3 C_{An} C_{Bn}$

dV = 0.05 (ft^3)

and at: $V_o = 0$, $C_A = C_{Ao}$

$V_1 = V_o + dV$, n = 0, $C_A = C_{A1}$

$V_2 = V_1 + dV$, n = 1, $C_A = C_{A2}$

…….

Repeat the steps for others component B, C, D, E

Due to the assumption of 99.99% conversion of ethylene oxide, we repeated the calculation in the Excel sheet from n = 0 to where $C_A \approx 0$.
Then we record the final values of C_B, C_C, C_D, C_E at $C_A \approx 0$ and convert the results from concentration back to molar flow rate, F_i, then mass flow rate.

2.3.3. Energy Balance

The operating condition of the reactor is at 401°F and 355.3 PSIG, so all of the components in the feeding stream can stay in liquid form at this temperature and pressure. The reaction is in the liquid phase so both temperature and pressure remained constant throughout the process. The steps used to simplify the general energy balance equation are shown in the ethylene epoxidation reactor calculation part and apply the same for ethylene glycol reactors. The amount of heat that needs to be removed shows in Table 2.
For this reactor, the equation rearranged to:

$$\dot{Q} = \Delta H_{Rx1} F_{Ao} X + \Delta H_{Rx2} F_{Co} X + \Delta H_{Rx3} F_{Do} X$$

At the outlet of the reactor, we have:

$$F_{Ao} X_A = F_C$$

$$F_{Co} X_C = F_D$$

$$F_{Do} X_D = F_E$$

$$\dot{Q} = \Delta H_{Rx1} F_C + \Delta H_{Rx2} F_D + \Delta H_{Rx3} F_E$$

$$\Delta H_{Rx1} = H_C^o - H_B^o - H_A^o + [(C_{PC} - C_{PB} - C_{PA}) * (T - T_R)]$$

$$\Delta H_{Rx2} = H_D^o - H_C^o - H_A^o + [(C_{PD} - C_{PC} - C_{PA}) * (T - T_R)]$$

$$\Delta H_{Rx3} = H_E^o - H_D^o - H_A^o + [(C_{PE} - C_{PD} - C_{PA}) * (T - T_R)]$$

If the recycle stream carried some of the products back into the reactor, we need to subtract the amount of the component in the recycle stream by its outlet flow rates because only the new production created heat. All of the $H_i^o \text{ and } C_{Pi}$ values are found based on the UH library [25], and the total energy that needed to be removed from the reactor can be calculated.

2.4. Separation of Ethylene Glycol Products

The EG reactor effluent runs through a separation train of 3 distillation columns; 2 focused on separating water (H2O Distillation Columns 1 and 2) and 1 on EG (MEG Column). All were designed using the Fenske-Underwood-Gilliland (FUG) shortcut method.

2.4.1. Assumptions

$$Fenske:$$

$$N_{min} = \frac{\ln\left(\frac{x_{HK,B}}{x_{LK,B}} \frac{x_{LK,D}}{x_{HK,D}}\right)}{\ln\left(\left[\alpha_{LK,HK}\right]_m\right)}$$

$$Underwood:$$

$$R_{min} = \left(\frac{L}{D}\right)_{min} = \frac{y_{HK,F} x_{LK,D} - y_{LK,F} x_{HK,D}}{y_{LK,F} x_{HK,F} - y_{HK,F} x_{LK,F}}$$

$$Gilliland:$$

$$X = \frac{R - R_{min}}{R + 1}$$

$$Y = \frac{(N - N_{min})}{N + 1} = 1 - \exp\left[\left(\frac{1 + 54.4X}{11 + 117.2X}\right)\left(\frac{X - 1}{X^{0.5}}\right)\right]$$

$$N = \frac{Y + N_{min}}{1 - Y}$$

The key assumptions for our methodology include the following:

- Solutions are ideal there allowing the use of Raoult's Law for calculating K-value
    - $K = \frac{P_S}{P}$
- Pressure drop of 2 psi across the reboiler and condenser
- All columns use a total condenser and partial reboiler
- Pressure drop of 3 psi across the column

Using Excel Solver and the FUG equations, we performed the following procedures to determine the characteristics of each distillation column:

2.4.2. H2O Distillation Columns:

1) We assumed values for the distillate recovery of each component in the feed and by trial-and-error calculated the expected distillate composition and cut point (fraction of total feed that goes to distillate).

$$x_{iD} = x_{iF} \frac{\frac{d_i}{f_i}}{\frac{D}{F}}$$

Constraints

$$\Sigma x_{iD} = 1$$
$$0 \leq x_{iD} \leq 1$$

2) With the distillate recoveries, composition, and cut point determined, we then assumed an overall operating pressure for the column.
    a. We assumed that the feed would always be a bubble-point liquid.
3) We solved for the flash temperatures of the feed, distillate, and bottoms at the column operating pressure as well as the feed flash liquid and vapor compositions.
    a. We defined an error function that Solver can work to minimize in trying to solve for the aforementioned variables.

    $$\epsilon = \epsilon_{Pressure} + \epsilon_{Composition}$$

    $\epsilon_{Pressure}$ represents the cumulative errors in the operating pressure and pressure calculated from the flash vapor mole fractions of the feed, distillate, and bottoms. $\epsilon_{Composition}$ is the cumulation of errors in the calculated flash vapor compositions (i.e. how close their sums equal 1).
4) Finally using the FUG equations written at the beginning of this section, we determine the remaining characteristics of the column such as a number of stages, reflux ratios, etc.

2.4.3. MEG Column:

1) Instead of determining the distillate compositions from assumed values of distillate recovery, we do the reverse in this step.
    a. We assumed that the distillate composition would match the target product specifications for MEG from the project statement.
    b. We also assumed the expected distillate recovery will equal 99% by assuming a loss of 1 % of the MEG in the feed stream.
2) By trial-and-error, we solve for the remaining distillate recoveries and cut point.

$$\frac{d_i}{f_i} = \frac{x_{iD}}{x_{iF}}\frac{D}{F}$$

Constraints

$$0 \leq \frac{d_i}{f_i} \leq 1, i \neq MEG$$

$$\frac{d_{MEG}}{f_{MEG}} = 0.99$$

3) After completing the preceding steps, we used the same assumptions and variables we manipulated in the previous procedure.
    a. The only exception is that the operating pressure is manipulated rather than assumed.
    b. We utilized the same error function used in the previous procedure.

2.5. Auxiliary Equipment

2.5.1. Pumps

2.5.1.1. Material Balance

$$\sum m_{in} = \sum m_{out}$$

The above equation is true for the mass balance of all the pumps.

2.5.1.2. Energy Balance

The simplified energy balance for a pump is as follows:

$$W_s = \Delta H$$

The shaft work for the operation of our pumps was calculated using the following equation:

$$W_{s\,(ideal)} = (\frac{1}{\rho})(P_2 - P_1)$$

$$W_s = \frac{W_{s\,(ideal)}}{\eta}$$

The procedure used to calculate the shaft work of each pump was to use the specific volume (or inverse of the density of the stream) and the pressure increase of the pump to obtain an ideal shaft work, and use the pumps specified efficiency of 85% to obtain an actual shaft work value. The density used for the calculations was a mass-weighted average of the components in each pump.

2.5.2. Compressor

2.5.2.1. Material Balance

$$\sum m_{in} = \sum m_{out}$$

The above equation is true for the mass balance of all compressors.

2.5.2.2. Energy Balance

The simplified energy balance for a compressor is as follows:

$$W_s = \Delta H$$

The shaft work required for the operation of our compressor was calculated by the following series of equations:

$$T_2' = T_1(\frac{P_1}{P_2})^{R/(C_p')_s}$$

$$(\Delta H)_s = W_{s\,(isentropic)} = \left(C_p'\right)_H (T_2' - T_1)$$

$$W_s = \frac{W_{s\,(isentropic)}}{\eta}$$

The procedure used to calculate the shaft work was first calculating an isentropic outlet temperature using both inlet and outlet pressures, and an isentropic mean heat capacity. This value was then used with the mean heat capacity to calculate an isentropic shaft work. The actual shaft work was finally calculated based on the isentropic efficiency of the compressor which we specified as 85%.

2.5.3. Heat Exchangers

2.5.3.1. Material Balance

$$\sum m_{in} = \sum m_{out}$$

The above equation is true for the mass balance of all the heat exchangers.

2.5.3.2. Energy Balance

H-1and H-3 has heat integration hence, Q = 0 for those heat exchangers.
To calculate the exiting temperature, an Excel solver was used to find temperatures that make Q = 0.

$$\frac{C_P}{R} = A + BT + CT^2 + DT^{-2} + ET^3 \, with\, T\, in\, K\, and\, C_p\, in\, \frac{KJ}{mol}$$

$$Q = \Delta H = mCpdt$$

Using mass flowrates and the above two equations to calculate temperatures and Q for the heat exchangers that aren’t integrated.

2.5.4. Valves

2.5.4.1. Material Balance

$$\sum m_{in} = \sum m_{out}$$

The above equation is true for the mass balance of all the valves.

2.5.4.2. Energy Balance

Valves are considered adiabatic for the entire plant. Lee Kesler correlations were used to calculate the exit temperatures of the throttling valves. Since ΔH for valves are zero, the entry and exit pressure are known and so is the entering temperature, the only unknown is the exit temperature which can be calculated through trial and error.

$$Z = Z^o + \omega Z^1$$

$$P_r = \frac{P}{P_c};$$

$$T_r = \frac{T}{T_c}$$

$$\Delta H = H_2 - H_1 = (H_1^o - H_1) + (H_2^o - H_1^o) + (H_2 - H_2^o)$$

3. Sizing & Cost

3.1. Pumps

3.1.1. Sizing

All the pumps have a centrifugal design as shown in Figure 1.

$$W_o = \frac{H\dot{m_v}\rho}{10^3}$$

To calculate the head of the pump, the above equation was used where, W_o is the shaft work of the pump in kW, $\dot{m_v}$ is the volumetric flowrate in m^3/s , and ρ is the liquid density in kg/m^3 [28]. Relevant conversion units were used to calculate the head of the pump in ft and all the other specifications were calculated through the values found in material balances.

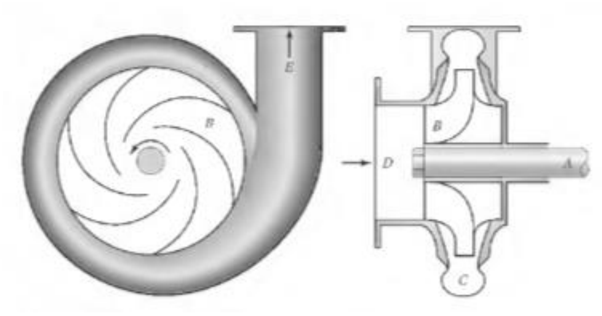


Figure 1 - centrifugal design

The material of Construction for each pump was chosen based on the species reactivity with certain metals.

3.1.2. Cost

Figure 2 was used to calculate the cost of the equipment and then the cost was adjusted to reflect the cost of the equipment today. The equation used was $Cost = (Base\ Cost) * \frac{I}{I_{base}}$ with I_{base} = 395.6 and I = 607.5 [35]. The cost of the individual pumps is reflected in Table 5.

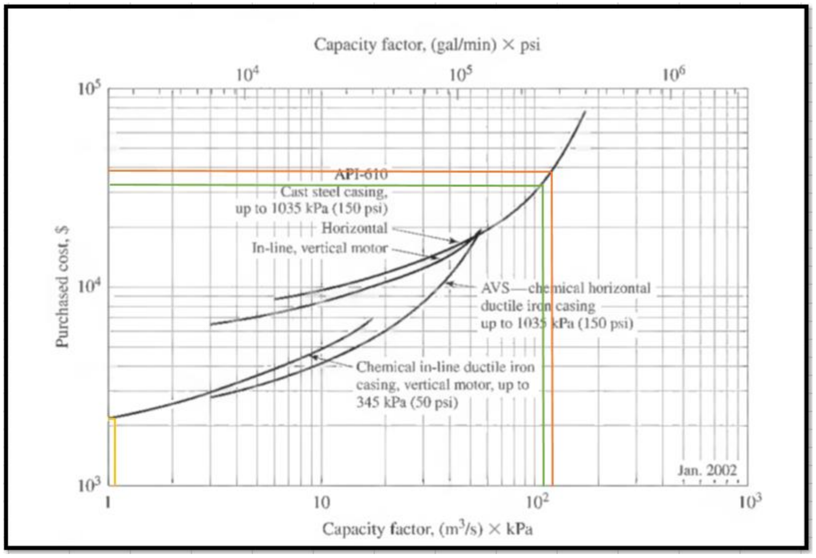


Figure 2 – Figure 12.20 from [28]. Cost for centrifugal pumps

Pump 1 (m^3/s)*kPa	110.7996609
Cost 2002, $	$ 31,000.00
Cost 2019, $	$ 47,604.90

Pump 2 (m^3/s)*kPa	134.1258146
Cost 2002, $	$ 39,900.00
Cost 2019, $	$ 61,272.12

Pump 3 (m^3/s)*kPa	1.171967244
Cost 2002, $	$ 2,100.00
Cost 2019, $	$ 3,224.85

Table 5 – Pump cost by capacity factor

3.2. Compressors

3.2.1. Sizing

The compressor has a centrifugal design as shown in Figure 1. The work of the compressor was calculated using the following equations:

$$T_2' = T_1\left(\frac{P_2}{P_1}\right)^{\frac{R}{C_p}}\ ;\ Ws(isentropic) = C_p(T_2' - T_1);\ Ws = \frac{Ws(isentropic)}{\eta_{isentropic}}$$

An efficiency of 85% is being assumed.

3.2.2. Cost

Figure 2 was used to calculate the cost of the compressor. The table on the right shows the cost of the compressor calculated and adjusted.

Compressor 1 (hp)	-2224.14
Cost 2002, $	$ 3,000,000.00
Cost 2019, $	$ 4,606,926.19

Table 6 – Compressor cost by capacity factor

3.3. Mixers & Splitters

3.3.1. Cost

Figure 3 was used to the cost of the mixers and the splitters. The volume was calculated using the mass flowrates and the density. For the vapor streams, the ideal gas equation was used and for liquid streams, constants were used from Perry’s Handbook and Knovel – online engineering toolbox.

The material of Construction for Mixer 1, Mixer2, Mixer 3, Vent Drum, and the Knockout Drum is Stainless Steel and Carbon Steel for Splitter 1, Splitter 2, and Splitter 3.

Table 7 shows the base cost calculated from the figure 3 and then adjusted using the formula: $Cost = (Base\ Cost) * \frac{I}{I_{base}}$ with I_{base} = 395.6 and I = 607.5 [35]. The cost of the individual's splitters and mixers is reflected in Table 7.

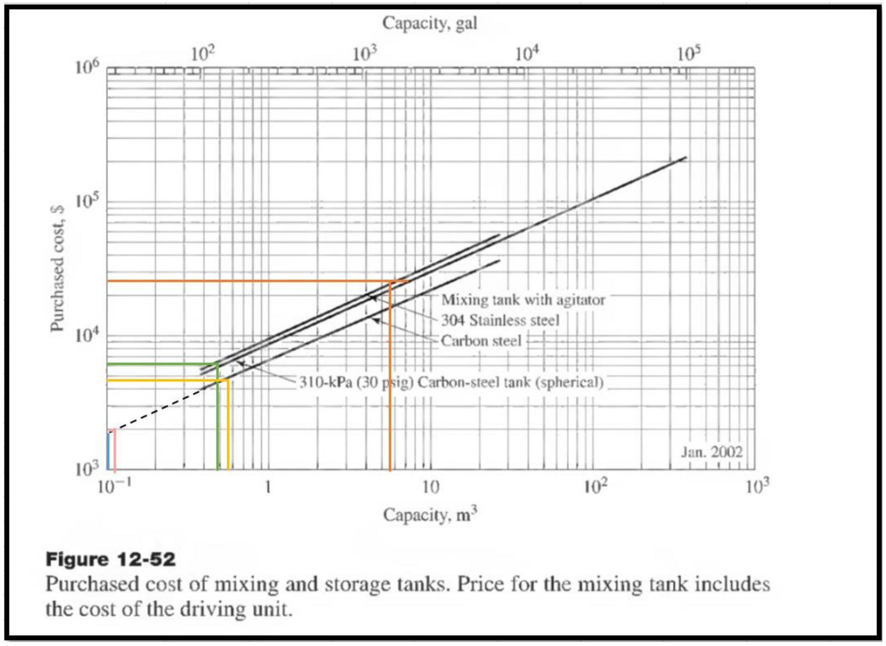


Figure 12-52
Purchased cost of mixing and storage tanks. Price for the mixing tank includes the cost of the driving unit.

Figure 3 – Figure 12-52 from [28]. Cost of mixing and storage tanks

Equipment	Base Cost 2002, $	$ Cost, 2019
Mixer 1	$ 26,000.00	$ 39,926.69
Mixer 2	$ 26,000.00	$ 39,926.69
Mixer 3	$ 6,000.00	$ 9,213.85
Splitter 1	$ 4,900.00	$ 7,524.65
Splitter 2	$ 200.00	$ 307.13
Splitter 3	$ 2,000.00	$ 3,071.28
Vent Drum	$ 26,000.00	$ 39,926.69

KO Drum	$ 26,000.00	$ 39,926.69

Table 7 – Cost of all mixers, splitters, and drums

3.4. Valves

3.4.1. Sizing

All valves are carbon steel globe valves (Figure 4) with the same diameter. Carbon steel is chosen because it is on the cheaper side of the materials of construction. The reason globe valves are chosen is that they are flexible with varying pressures. The diameter was chosen to be the median recorded diameter in Figure 6 which is 0.1042 ft.

Figure 4 – carbon steel globe valves

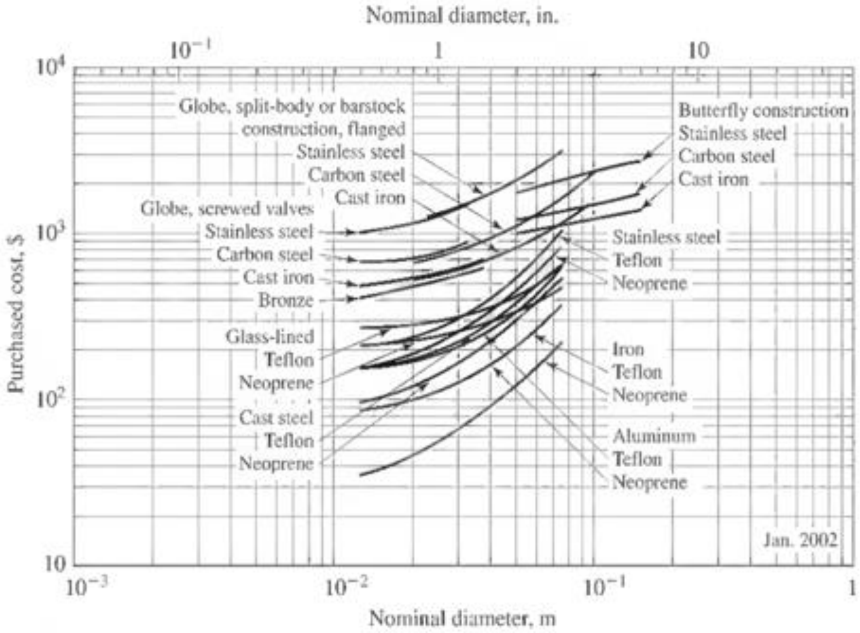


Figure 12-10
Purchased cost of diaphragm valves

Figure 5 – Figure 12-10 from [28] detailing cost of valves based on type, material, and nominal diameter

3.4.2. Cost

Using Figure 5 and the nominal diameter, the cost of the valves was determined. Table 8 shows the base cost calculated and then adjusted using the formula: $Cost = (Base\ Cost) * \frac{I}{I_{base}}$ with I_{base} = 395.6 and I = 607.5 [35].

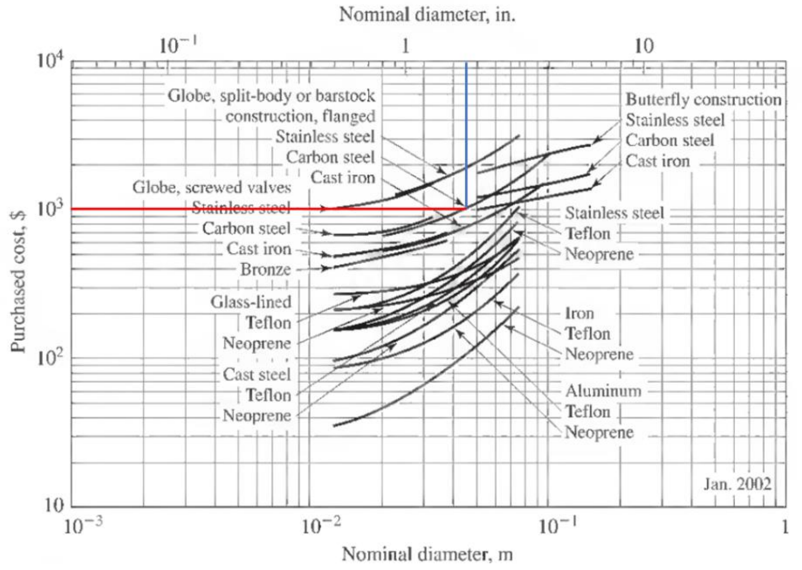


Figure 12-10
Purchased cost of diaphragm valves

Figure 6 – The median nominal diameter for globe carbon steel was chosen as the standard diameter for all valves used in process

Valve	Nominal diameter (in.)	Cost (2002) ($)	Final Cost
V-1	1.25	$ 1,050.00	$ 1,612.42
V-2	1.25	$ 1,050.00	$ 1,612.42
V-3	1.25	$ 1,050.00	$ 1,612.42
V-4	1.25	$ 1,050.00	$ 1,612.42
V-5	1.25	$ 1,050.00	$ 1,612.42
V-6	1.25	$ 1,050.00	$ 1,612.42

Table 8 – Cost of valves used

3.5. Absorbers and Strippers

3.5.1. Sizing

There are 2 absorbers: EO Scrubber and CO_2 Scrubber and one stripper: EO Desorber and they are modeled as sieve tray column (Figure 7). If $0.2 < \mu_L < 1.6$ cP then efficiency can be calculated using the equation: $E_0 = 19.2 - 57.8 log \mu_L$. If the μ_L does not fall in the range, efficiency can be calculated using the following equation:

$$logE_0 = 1.597 - 0.199\log\left(\frac{KM_L\mu_L}{\rho_L}\right) - 0.0896\left(\log\left(\frac{KM_L\mu_L}{\frac{\rho_L}{16.02}}\right)\right)^2 .$$

An actual number of trays can be calculated then by using the equation: $N_{act} = N/E_0$ [28].

Column height was calculated using the equation, $H_c = (N_{act} - 1)H_s + \Delta H$, where H_s is the tray spacing and ΔH is the height needed above the first tray for liquid removal and below the last tray for bottom surge capacity. For these calculations, the tray spacing for all the columns in 12 ft and ΔH is 14 ft [30].

Flooding fraction (F_f) was chosen to be 0.8 and the surface tension was assumed to be 70. Both are simplifying assumptions based on the values used widely.

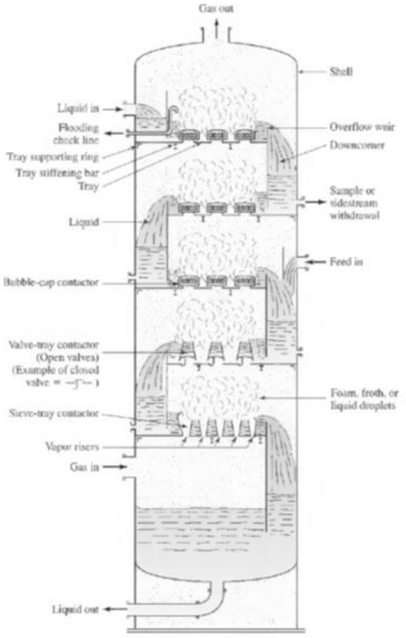


Figure 15-2
Cross-sectional view of a finite-stage contactor column in operation showing an example of a sieve tray, a valve tray, and a bubble-cap tray

Figure 7 – Sieve tray column

To calculate the diameter of the column, the following equations were used:

$$D = (4A_c/\pi)^{\frac{1}{2}} \quad ; \quad A_c = A_n + A_d \quad ; \quad A_n = \frac{\dot{m}_v}{V_n}$$

$$V_{nf} = C_{sb}\left(\frac{\sigma}{20}\right)^{0.2}\left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{0.5} \quad ; \quad V_n = F_f * V_{nf}$$

C_{sb} can be calculated using Figure 8 based on the equation: $F_{LV} = \left(\frac{L}{V}\right)(\rho_V/\rho_L)^{0.5}$ [28].

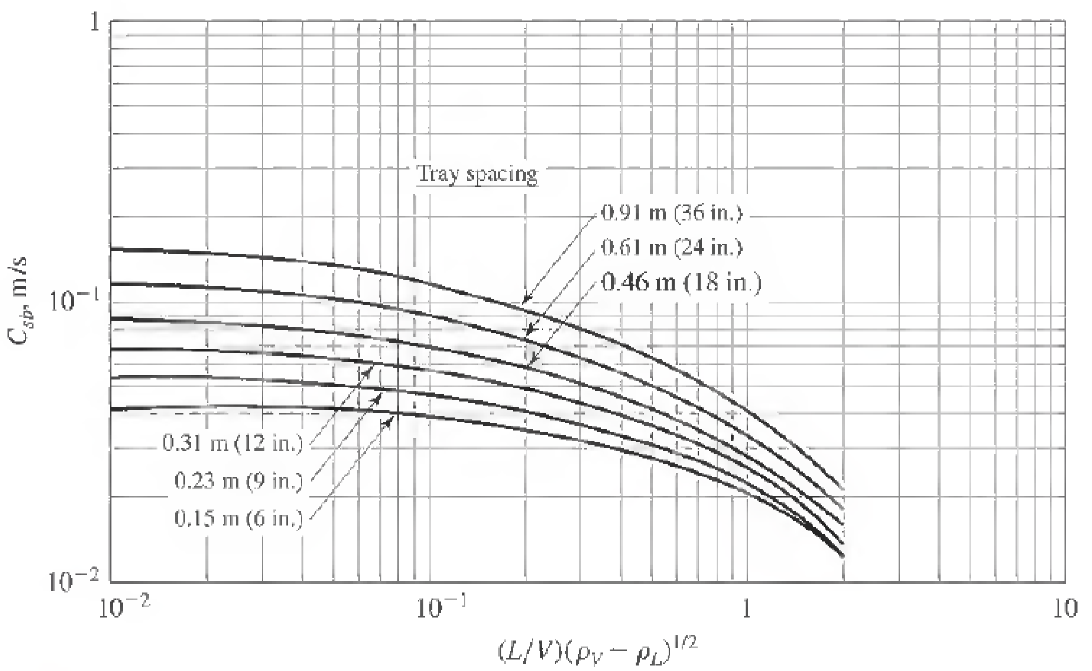
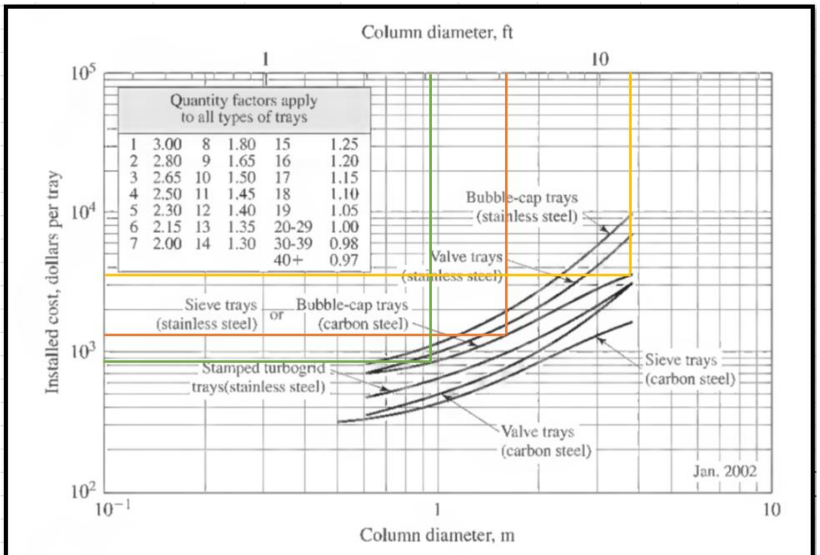


Figure 8 – Figure 15-5 from [28] used for determining C_{SB} and tray spacing

3.5.2. Cost

Once the diameters of the columns are calculated, Figure 9 was used to find the cost of each tray. Table 9 shows the individual costs of each column where the base cost is adjusted using the formula: $Cost = (Base\ Cost) * \frac{I}{I_{base}}$ with I_{base} = 395.6 and I = 607.5 [35].



Quantity factors apply to all types of trays

1	3.00	8	1.80	15	1.25
2	2.80	9	1.65	16	1.20
3	2.65	10	1.50	17	1.15
4	2.50	11	1.45	18	1.10
5	2.30	12	1.40	19	1.05
6	2.15	13	1.35	20-29	1.00
7	2.00	14	1.30	30-39	0.98
				40+	0.97

Figure 15-13

Purchased cost of trays in tray columns. Price includes tray deck, bubble caps,

Figure 9 – Figure 15-13 from [28] used to determine cost/tray based on material and type

Column Height (ft)		1/2 (ft)	1/2 $ / tray	$ / tray	$ Base Cost, 2002	$ Cost, 2020
EO Scrubber	16.297	8.14872684	1400	2800	$ 109,490.48	$ 168,138.18
EO Desorber	16.353893	8.17694648	850	1700	$ 107,384.89	$ 164,904.75
CO2 Scrubber	21.453969	10.7269845	3700	7400	$ 484,155.23	$ 743,489.13

Table 9 – Cost of the absorbers and strippers based on total tray cost

3.6. Reactor 1 & Reactor 2

3.6.1. Sizing

- **Reactor 1**

For the ethylene oxide reactor, the reactor acted like a heat exchanger. So, the method to determine the heat exchanger size will apply here as well. Since the reactions are exothermic, a shell-and-tube reactor design is ideal because it allows for coolant to be run through the shell side for heat exchange. This is critical in reducing hot spot formation, and more importantly in preventing the reactor temperature from running away. The process feed flows through the tube side, while the cooling water flows through the shell side. The reactors are vertical to provide backpressure for the system. This helps to keep the catalyst in place. We used the mean log method shows below with all of the information in Table 10 to find the heat exchange area. Then based on the calculated heat exchange area, we choose a tube length that was in the given range (6 -10 m) and found all of the dimensions needed to construct the reactor.

$$\dot{Q} = U_o \cdot A \cdot LMTD$$

Rearrange,

$$A = \frac{\dot{Q}}{U_o \cdot LMTD}$$

$$LMTD = \frac{\Delta T_A - \Delta T_B}{ln\left(\frac{\Delta T_A}{\Delta T_B}\right)}$$

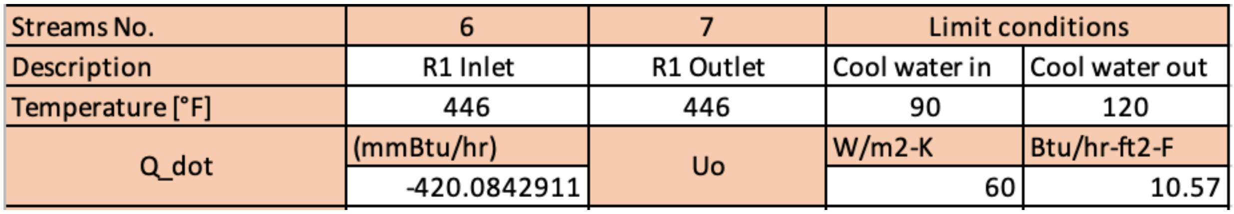
Co-current:

$$\Delta T_A = T_{shell\_in} - T_{tube\_in}$$
$$\Delta T_B = T_{shell\_out} - T_{tube\_out}$$

Countercurrent:

$$\Delta T_A = T_{shell\_in} - T_{tube\_out}$$

$$\Delta T_A = T_{shell\_out} - T_{tube\_in}$$



Streams No.	6	7	Limit conditions	
Description	R1 Inlet	R1 Outlet	Cool water in	Cool water out
Temperature [°F]	446	446	90	120
Q_dot	(mmBtu/hr)	Uo	W/m2-K	Btu/hr-ft2-F
	-420.0842911		60	10.57

Table 10 – Reactor 1 inlet and outlet stream conditions

- **Reactor 2**

The sizing for reactor 2 is much simpler. We used Euler's method to calculate the mass balance for reactor 2. By targeting the conversion of ethylene oxide to be 99.99%, we found the required volume value, which is 937.6 ft3. Then based on the literature, we choose our tube diameter to be 1.97 ft then calculate the reactor 2 length based on the cylinder volume equation. It turned out to be a long reactor.

$$V = \pi r^2 L$$

3.6.2. Cost

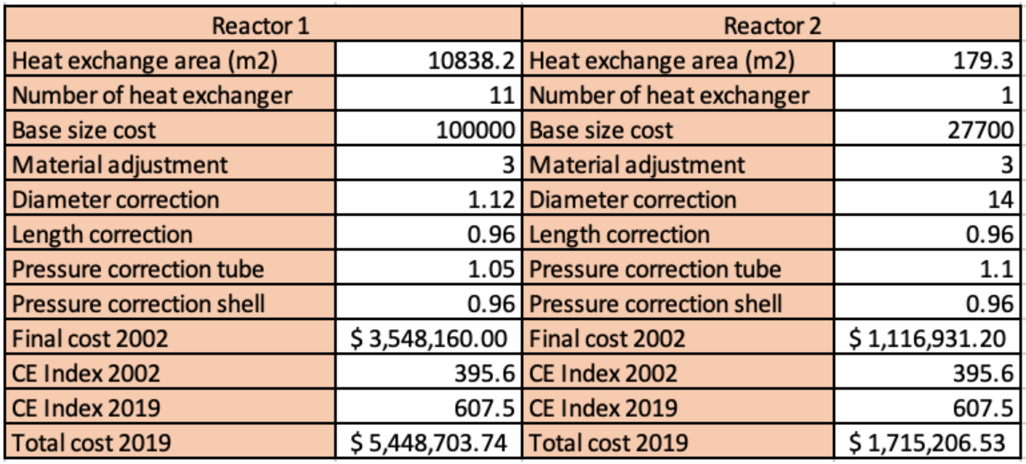
Because both reactors are acting like heat exchangers, we will have to calculate the cost base on the heat exchange areas. Even though carbon steel is stronger, it is high in carbon that when exposed to moisture can corrode and rush quickly [11]. Ethylene oxide is very reactive with rust; the use of stainless steel is critical to avoid a hazardous situation. Moreover, stainless steel is designed to protect against oxidization, so we choose to use stainless steel for both shells and tubes of the reactors. The final cost of the reactors is found by using the equation below combine with the values in Table 11 extracted from Figures 10-13.

$$\begin{aligned} Final\ cost = {} & base\ cost * number\ of\ HE * adjustment * diameter\ correction \\ & * length\ correction * pressure\ correction\ tube\ side \\ & * pressure\ correction\ shell\ side \end{aligned}$$

The final cost was then adjusted using the formula:

$$Cost = (Base\ Cost) * \frac{I}{I_{base}}$$

with I_{base} = 395.6 and I = 607.5.



Reactor 1		Reactor 2	
Heat exchange area (m2)	10838.2	Heat exchange area (m2)	179.3
Number of heat exchanger	11	Number of heat exchanger	1
Base size cost	100000	Base size cost	27700
Material adjustment	3	Material adjustment	3
Diameter correction	1.12	Diameter correction	14
Length correction	0.96	Length correction	0.96
Pressure correction tube	1.05	Pressure correction tube	1.1
Pressure correction shell	0.96	Pressure correction shell	0.96
Final cost 2002	$ 3,548,160.00	Final cost 2002	$ 1,116,931.20
CE Index 2002	395.6	CE Index 2002	395.6
CE Index 2019	607.5	CE Index 2019	607.5
Total cost 2019	$ 5,448,703.74	Total cost 2019	$ 1,715,206.53

Table 11. Cost analysis for both reactors

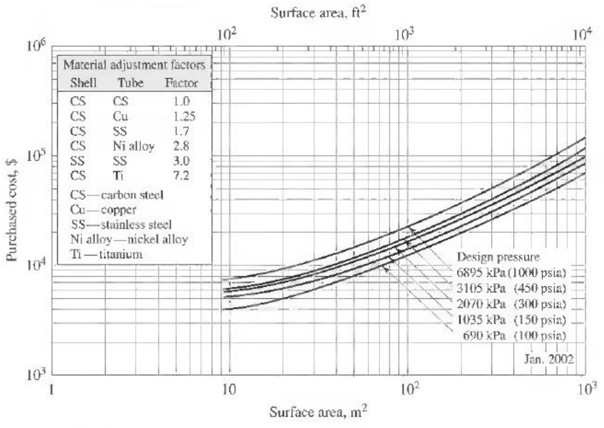


Figure 14-19
Purchased cost of floating-head heat exchangers with 0.019-m OD × 0.025-m ($\frac{3}{4}$-in. OD × 1-in.) square pitch and 4.88-m (16-ft) bundles of carbon-steel construction

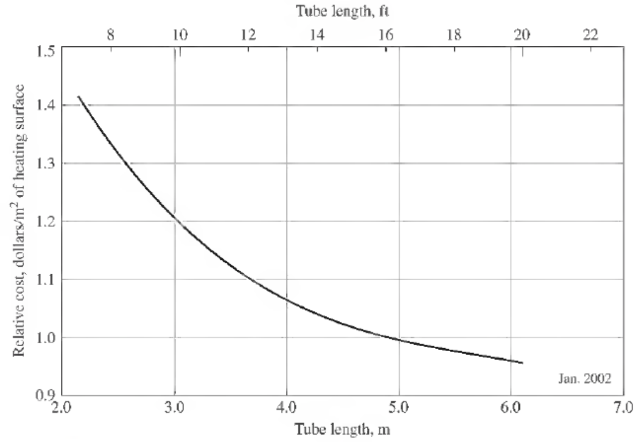


Figure 14-22
Effect of tube length on cost of conventional shell-and-tube heat exchangers

Figure 10. Base cost

Figure 11. Length correction ratio

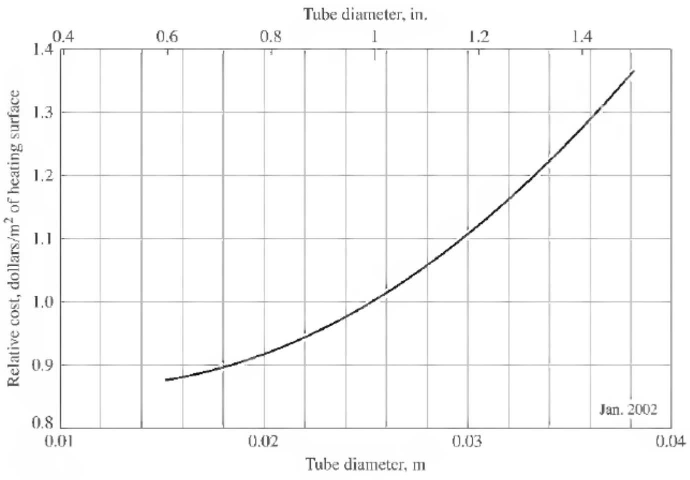


Figure 14-21
Effect of tube diameter on cost of conventional shell-and-tube heat exchangers

Figure 12 – Diameter Correction Ratio

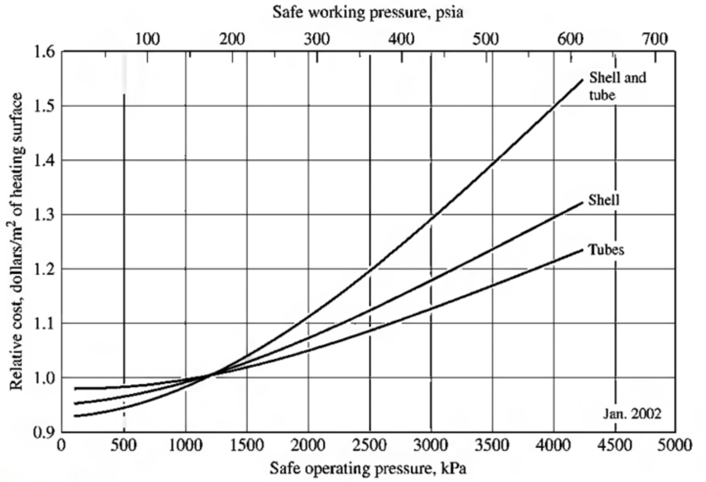


Figure 14-23
Effect of operating pressure on cost of conventional shell-and-tube heat exchangers

Figure 13 - Pressure correction ratio

3.7. H2O Distillation & MEG Columns

3.7.1. Sizing

We sized the distillation columns similarly to how we sized the absorbers and strippers. However, instead of using column efficiency to compute the number of stages, we used numbers computed from the Gilliland equations for each column. Furthermore, we assumed tray spacing to be 2 ft rather than 1 because our source for distillation cost estimation used this spacing in their content.

3.7.2. Cost

We used the following expressions from "Chemical Engineering Design - Principles, Practice and Economics of Plant and Process Design" [34] to determine the cost of each column:

Column	Total Cost
Evaporator 1	$5,929,152.53
Evaporator 2	$360,368.52
MEG	$2,522,797.93

Table 12 – Final cost of distillation columns. Values have been scaled based on the CE Index [35]

$$Total\ Cost\ =\ Shell\ purchase\ cost\ +\ Shell\ installation\ cost\ +\ Tray\ installation\ cost$$

$$Shell\ purchase\ cost\ =\frac{M\ \&\ S\ Index\ (2011)}{280}\ (957.9D^{1.066}H^{.802}F_C)$$

$$Shell\ installation\ cost=\frac{M\ \&\ S\ Index\ (2011)}{280}\ (957.9D^{1.066}H^{.802})(2.18+F_C)$$

$$F_C=F_mF_P$$

$$F_m=3.67\ (solid\ stainless\ steel)$$

$$F_P = 1 + 0.0074(P - 3.48) + 0.00023(P - 3.48)^2$$

$$Tray\ installation\ cost\ (per\ tray) = \frac{M\ \&\ S\ Index\ (2011)}{280}\ (97.2D^{1.55}HF_C)$$

$F_C = F_t + F_m$

$F_t = 0\ (sieve\ tray)$

$F_m = 1.7\ (stainless\ steel)$

3.8. Heat Exchangers

3.8.1. Sizing

For heat exchanger sizing, we utilized the following equation:

$$Q = U * A * \Delta T_{LMTD}$$

Where,

U = Overall heat transfer coefficient

A = Heat exchange area

ΔT_{LMTD} = Log mean temperature difference = $\frac{\Delta T_1 - \Delta T_2}{\ln(\frac{\Delta T_1}{\Delta T_2})}$

To obtain U values, table 14-5 from our design textbook [28] was used, with the U value depending on the type of fluid on each side of the exchanger. Using this equation, we were able to obtain our heat exchange area which was the characteristic length used to estimate the cost of the exchanger.

3.8.2. Cost

For cost estimation of our exchangers, we utilized the heat exchange area found when sizing them, along with their material of construction and figure 13 to obtain a 2002 cost estimate.

Once we had a base 2002 cost, we were able to use the following equation to obtain a present-day cost estimate for our heat exchangers.

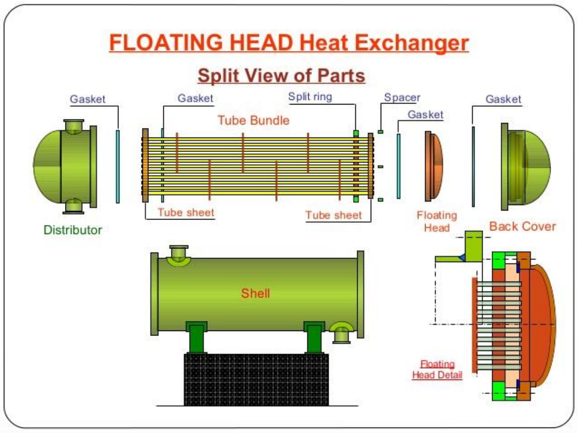


Figure 12 - Floating Head Heat Exchanger

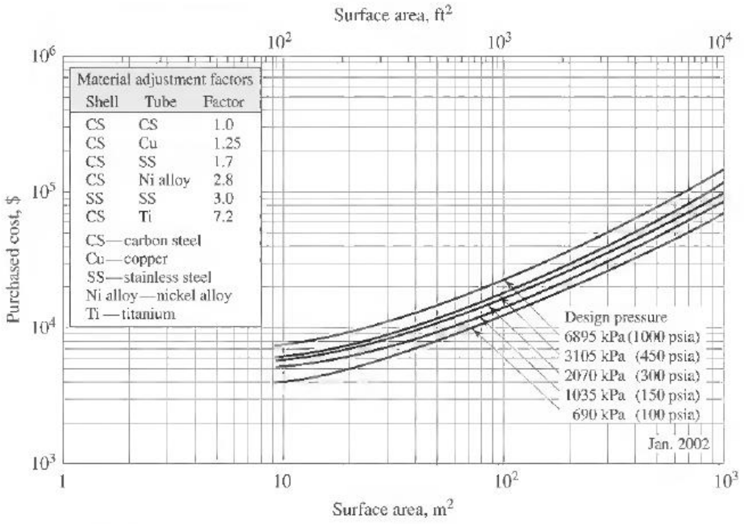


Figure 14-19
Purchased cost of floating-head heat exchangers with 0.019-m OD × 0.025-m ($\frac{3}{4}$-in. OD × 1-in.) square pitch and 4.88-m (16-ft) bundles of carbon-steel construction

Figure 13 – Cost of floating-head heat exchangers based on surface area

$Cost = (Base\ Cost) * \frac{I}{I_{base}}$ with I_{base} = 395.6 and I = 607.5.

For some exchangers where the heat exchange area is very small, the cost of the exchanger was taken to be the minimum value for the respective curve based on the process stream pressure. This was done as it was assumed that there is a minimum cost to fabricate a heat exchanger regardless of the size of the equipment.

3.9. Utilities

3.9.1. Cooling Water

3.9.1.1. An average cost per cubic ft was derived from Table 13. Assuming a density value of approximately 1000 kg/m^3, we calculated the cost of each cooling water supply used in the process and scaled the result according to the CE Index [35].

3.9.2. Steam

3.9.2.1. We used the following equation from “Chemical Engineering Design - Principles, Practice and Economics of Plant and Process Design” [31] to determine the cost of both MP and HP steam:

$$P_{HPS} = P_F \frac{dH_b}{\eta_B} + P_{BFW}$$

$$P_{HPS} = price\ of\ HP\ or\ MP\ steam\ (\frac{\$}{Mlb})$$

$$P_F = price\ of\ fuel\ \left(\frac{\$}{MMBtu}\right)$$

$$dH_b = heating\ rate\ (\frac{MMBtu}{Mlb})$$

$$\eta_B = boiler\ efficiency$$

$$P_{BFW} = price\ of\ boiler\ feed\ water\left(\frac{\$}{Mlb}\right)$$

Several factors determined the variables above, and they are listed in Table 14.

3.9.3. Amine Solution (Monoethanolamine)

3.9.3.1. We used the median value of the cost range presented in one of our sources [21] which was \$50/ton CO_2 captured.

Cooling Water Cost Reference		
Source	Cost Range (\$/m^3)	
Well	0.05	0.22
River/salt	0.02	0.06
Tower	0.02	0.07

Table 13 – Cost ranges for different sources of water [28]

Steam Cost Reference		
Variable	Value	References
Boiler Efficiency	0.9	31
BFW Cost (\$/1000 lb)	0.5	31
Assumed Fuel	Fuel oil no. 6	
Fuel Cost (\$/m^3)	163	28
Fuel Heating Value (Btu/lb)	18270	14
Approximate Density (lb/gal)	7.7	23
Approximate Density (lb/m^3)	2034.12	
Fuel Cost (\$/Btu)	4.39-06	
Fuel Cost (\$/MMBtu)	4.39	

Table 14 – Reference variables for calculating steam.

3.10. Raw Materials

The cost of ethylene was determined by multiplying the amount of fresh ethylene feedstock by the cost per pound of ethylene found in the source mentioned in Table 15. The cost of oxygen per cubic foot was determined by dividing the total value of oxygen shipped in the US in 2005 by the total volume of the oxygen shipped that same year.

Methane's cost was derived from the average industrial natural gas price in 2020. The data came from [10], and the natural gas price was scaled according to the assumed mole fraction of methane listed in Table 15.

Raw Material Costs		
Variable	Value	References
$/lb ethylene	0.33	26
Total volume of oxygen (2003)	103,070 × 10^6 ft^3	22
Total value of oxygen (2003)	$232,137 × 10^3	22
Approximate mole fraction of methane in natural gas	.947	1
Average industrial natural gas $/1000 ft^3	2.86	10

Table 15 – Reference variables for calculating raw material costs

4. Health, Safety & Environmental

4.1. Overview

Chemical manufacturing plants are full of potential threats to the safety of employees. Every day workers in chemical plants are exposed to hazardous chemicals, which may lead to serious injuries or even death. OSHA's Hazard Communication Standard (HCS) is based on a simple concept that employees have both a need and a right to know the hazards and identities of the chemicals they are exposed to when working [6].

Getting to know more about the toxicity, flammability, reactivity, and how to store and handle the chemical that they are working with is a way to reduce the risk of accidents. Although safety regulations are used primarily to keep employees from suffering serious injuries, they serve other purposes, too. For example, the employee will feel valued by their employers when they know that their safety is important. Additionally, safety procedures make sure that chemical plant workers can return to work the next day. Safety procedures help companies stay productive by avoiding accident-related shutdowns and other unnecessary interruptions.

While the feedstocks, ethylene and oxygen, and the final products, MEG, DEG, and TEG, of our process, are not extremely hazardous, a substance produced from the ethylene epoxidation reactor, ethylene oxide, can cause multiple serious health hazards. Ethylene oxide is toxic if inhaled, serious eye and skin irritation if exposed, and also may cause genetic defects, cancer, and frostbite. Proper PPE such as long pants, safety glasses, gloves, closed-toe shoes, and must be worn when working with these substances.

Some equipment throughout the plant is operated at extremely high temperatures and/or pressures. Compressed gases can cause fires, explosions, toxic gas exposures as well as the innate physical hazard associated with equipment under high pressure. All employees at a manufacturing plant should have a proper skill set, as well as knowledge on operating and handling the equipment under high temperature and pressure. Necessary training must be given to those who are responsible for repairing, maintaining, installing, or checking the pressure of the equipment.

All information on the potential hazards and how to work safely with the chemical product were documented on a Material Safety Data Sheet (MSDS). The MSDS contains much more information about the material than the label. It also shows us how to use and handling the product safely, what to do if accidents occur, and how to recognize symptoms of overexposure. Employees must read the MSDS before performing any action on the material. The MSDSs for all chemicals used in our design process is attached in Appendix 5 of this report.

4.2. Toxicity

Table 16 shows the permissible exposure limit for all the chemicals involved in the process. These values were determined by OSHA [8], and they are calculated based on 8-hour time-weighted averages.

Chemical	Permissible Exposure Limit (ppm)
Argon	N/A
Carbon Dioxide	5000
Diethylene Glycol	N/A
Ethane	N/A
Ethanolamine	3
Ethylene	N/A
Ethylene Glycol	N/A
Ethylene Oxide	1

Methane	N/A
Oxygen	N/A
Triethylene Glycol	N/A
Water	N/A

Table 16 - Permissible exposure limit

4.3. Flammability

To prevent a fire from happening, one of the three sides of the fire triangle (oxygen, fuel, and ignition source) needs to be eliminated. To make ethylene oxide, oxygen is required. So, there is no such way to eliminate the oxygen out of the process. Ignition sources are too many and very difficult to eliminate. The primary control method should be to prevent the existence of flammable mixtures.

Flammability limits are the most important characterization of gases and vapors hazards. A flammability diagram is an excellent way to represent the flammability of the mixture. To construct the diagram, flammability properties for all chemical species that we have to deal with are needed as shown in Table 17.

Species	Flammability	LFL (vol%)	UFL (vol%)	Auto-Ignition Temp (F)	Flash Point Temp (F)	Lower heat of combustion (KJ/mol)	Upper heat of combustion (Kj/mol)
Argon	NON-FLAMMABLE GAS						
Carbon Dioxide	NON-FLAMMABLE GAS						
Ethane	4	3	12.5	959	-211	-1428.6	-1559.8
Ethylene	4	2.7	36	842	-213	-1322.6	-1411.2
Ethylene Oxide	4	3	N/A	804	-67	-1218	-1264
Oxygen	NON-FLAMMABLE GAS						
Water	N/A						
Methane	4	5	15	1112	-306	-802.3	-890.3

Table 17. Flammability properties

Although oxygen itself is nonflammable, materials that burn in air will burn much more vigorously and at a higher temperature in an oxygen-enriched area. Below are equations that were used to construct our flammability diagram and the result are shown in Table 18 for flows that contained oxygen with flammable gases.

$$LFL_{mix\_o} = \frac{1}{\sum_i^n \frac{y_i}{LFL_{io}}}$$

$$UFL_{mix\_o} = \frac{1}{\sum_i^n \frac{y_i}{UFL_{io}}}$$

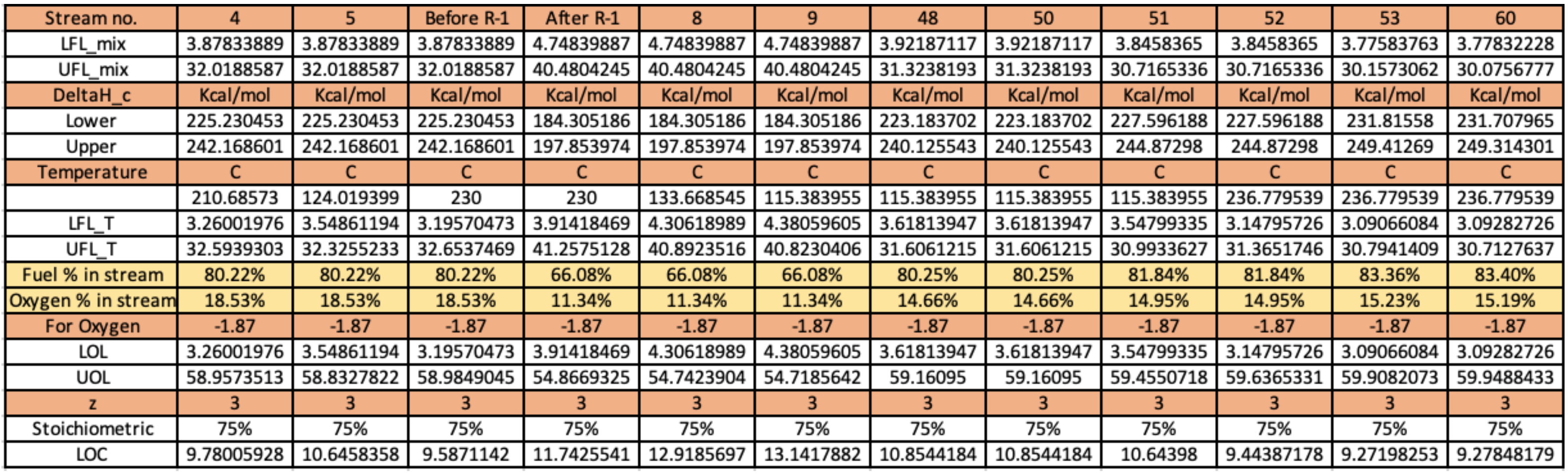
$$LFL_T = LFL_{mix\_o} \frac{0.75}{\Delta H_c}(T - 25)$$

$$UFL_T = UFL_{mix\_o} \frac{0.75}{\Delta H_c}(T - 25)$$

$$UOL = \frac{UFL_T\left[100 - C_{UOL}\left(100 - UFL_{mix\_o}\right)\right]}{UFL_{mix\_o} + UFL(1 - C_{UOL})}$$

$$LOC = z * LFL$$

$$Stoichiometric\ line = 100 * \left(\frac{z}{1 + z}\right)$$



Stream no.	4	5	Before R-1	After R-1	8	9	48	50	51	52	53	60
LFL_mix	3.87833889	3.87833889	3.87833889	4.74839887	4.74839887	4.74839887	3.92187117	3.92187117	3.8458365	3.8458365	3.77583763	3.77832228
UFL_mix	32.0188587	32.0188587	32.0188587	40.4804245	40.4804245	40.4804245	31.3238193	31.3238193	30.7165336	30.7165336	30.1573062	30.0756777
DeltaH_c	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol	Kcal/mol
Lower	225.230453	225.230453	225.230453	184.305186	184.305186	184.305186	223.183702	223.183702	227.596188	227.596188	231.81558	231.707965
Upper	242.168601	242.168601	242.168601	197.853974	197.853974	197.853974	240.125543	240.125543	244.87298	244.87298	249.41269	249.314301
Temperature	C	C	C	C	C	C	C	C	C	C	C	C
	210.68573	124.019399	230	230	133.668545	115.383955	115.383955	115.383955	115.383955	236.779539	236.779539	236.779539
LFL_T	3.26001976	3.54861194	3.19570473	3.91418469	4.30618989	4.38059605	3.61813947	3.61813947	3.54799335	3.14795726	3.09066084	3.09282726
UFL_T	32.5939303	32.3255233	32.6537469	41.2575128	40.8923516	40.8230406	31.6061215	31.6061215	30.9933627	31.3651746	30.7941409	30.7127637
Fuel % in stream	80.22%	80.22%	80.22%	66.08%	66.08%	66.08%	80.25%	80.25%	81.84%	81.84%	83.36%	83.40%
Oxygen % in stream	18.53%	18.53%	18.53%	11.34%	11.34%	11.34%	14.66%	14.66%	14.95%	14.95%	15.23%	15.19%
For Oxygen	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87	-1.87
LOL	3.26001976	3.54861194	3.19570473	3.91418469	4.30618989	4.38059605	3.61813947	3.61813947	3.54799335	3.14795726	3.09066084	3.09282726
UOL	58.9573513	58.8327822	58.9849045	54.8669325	54.7423904	54.7185642	59.16095	59.16095	59.4550718	59.6365331	59.9082073	59.9488433
z	3	3	3	3	3	3	3	3	3	3	3	3
Stoichiometric	75%	75%	75%	75%	75%	75%	75%	75%	75%	75%	75%	75%
LOC	9.78005928	10.6458358	9.5871142	11.7425541	12.9185697	13.1417882	10.8544184	10.8544184	10.64398	9.44387178	9.27198253	9.27848179

Table 18. Flammability diagram calculation

So, the two main streams that need to scrutinize their flammability limit are the stream before entering the first reactor and the stream exiting the first reactor. Based on Table 18, we have constructed the flammability diagram. As shown in Figure 14, we are trying to set the condition for all of our streams to avoid the flammable region. Flammability limits flame propagation will not be supported if fuel concentrations are either below the lower flammable limit (LFL) or above the upper flammable limit (UFL) in an oxidizing atmosphere. However, concentrations of mixtures in between these two limits, the two orange lines, will result in the formation of a flammable atmosphere, and possible fire or explosion could occur. The limiting oxygen concentration (LOC) is the minimum amount of oxygen needed to support flame propagation. Any gas mixture containing oxygen below the LOC is not flammable. LOL stands for lower oxygen limit and UOL stands for upper oxygen limit.

The black dots on the flammability diagram stand for the condition of our streams. As the result, all of our stream conditions are located outside the flammable region and safe to operate.

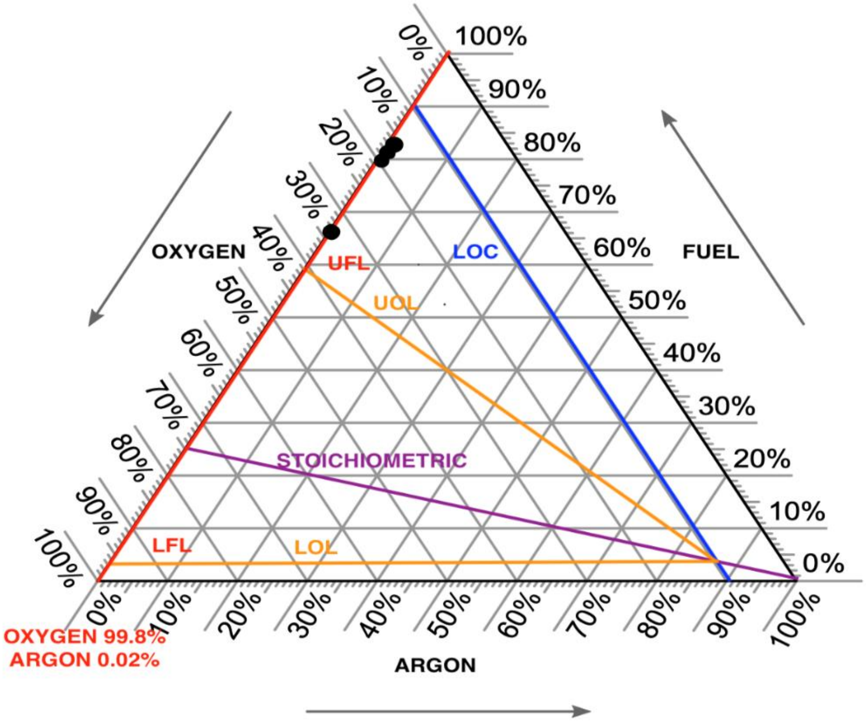
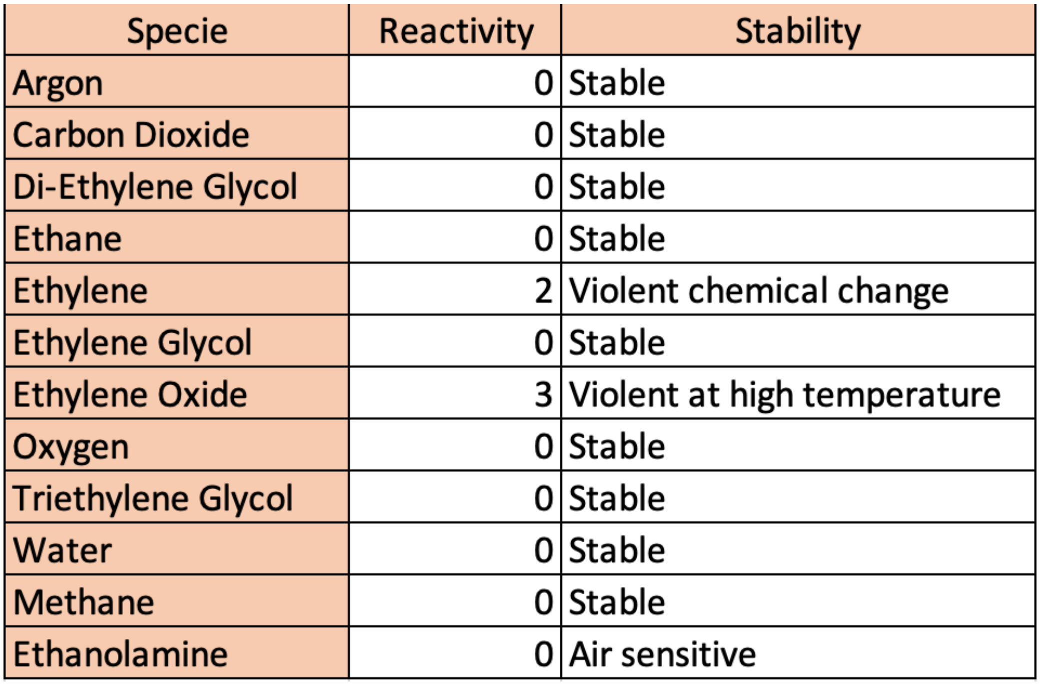


Figure 14. Flammability diagram

4.4. Reactivity

Reactivity is a measure of how readily a substance undergoes a chemical reaction. Highly reactive chemicals may undergo vigorous, uncontrolled reactions. When chemical reactions are not properly managed, they can have harmful, or even catastrophic consequences, such as toxic fumes, fires, and explosions [2]. These reactions may result in death and injury to people, damage to physical property, and severe effects on the environment. Species with high reactivity are called “unstable”, and species with low reactivity are called “stable”. It is important to recognize the reactivity of chemical compounds, as shown in Table 19, that will be used to avoid the incident from happening.



Specie	Reactivity	Stability
Argon	0	Stable
Carbon Dioxide	0	Stable
Di-Ethylene Glycol	0	Stable
Ethane	0	Stable
Ethylene	2	Violent chemical change
Ethylene Glycol	0	Stable
Ethylene Oxide	3	Violent at high temperature
Oxygen	0	Stable
Triethylene Glycol	0	Stable
Water	0	Stable
Methane	0	Stable
Ethanolamine	0	Air sensitive

Table 19.Substances' reactivity

4.5. Emissions

This plant has five types of exit streams: purge stream, waste-water removal streams, CO2 rich stream, MEG rich stream, which is our main product, and then DEG and TEG rich stream which are two main by-products.

The wastewater and CO2 rich streams will be sent to their respective treatment facilities. However, the vent stream is purging out 1 % of the feed stream hence a flare will be needed to burn hydrocarbon gases to ensure safety.

4.6. Environmental

Two major environmental concerns with the plant will be air pollution and waste-water treatment. Since there are substances part of the plant that are hazardous and can cause damage when inhaled or have been come in contact.

One such substance is ethylene glycol since it breaks down very rapidly in the air with a half-life of 8-84 hours and a much faster breakdown in soil with a half-life of 2-12 days. Hence, it is important to have devices and programs installed to check for any potential leaks. This preventative measure can be extended for all the hazardous chemicals to prevent any major catastrophe.

To combat the issue of waste-water treatment, there is a plan to build a waste-water treatment facility with a plant to treat the water before having it exit the facility. This will cost roughly about $8,909,900, which is below the projected amount for the outside battery limits.

5. Results and Discussion

5.1. Overview

For every process cycle, 105,044 lbm/hr of ethylene combined with 97,541 lbm/hr of oxygen creates 126,923 lbm/hr ethylene oxide. This amount of pure ethylene oxide then mixed with 1,075,702 lbm/hr of water to create 170,622 lbm/hr of MEG, 4,713 lbm/hr of DEG, and 118 lbm/hr of TEG. Based on the result, 96.7% of reacted ethylene oxide goes to produce MEG and around 3.3% to the byproducts, DEG and TEG.

After the separation process to achieve 99.9% of pure MEG, 0.05% of DEG, and 0.05% of water which meets our product specifications. These percentages are so exact because Excel Solver was used to calculating these values, and the output weight compositions were kept constant.

168,579 lbm/hr of MEG was retrieved as the final product for a plant whose operating hours are limited to 8,400 hours per year. Our chemical plant has achieved the total production quantity and product quality and can produce about 708-kilo tons of MEG per year, which is 1.15% above the target value.

Section 5.3 provides specifics for the mass balances and section 5.4 talks about the energy and work requirement of each equipment as well as the overall energy and work requirement.

Section 5.5 provides the specifics for each piece of equipment outlining the material of construction and major design specifications.

Section 5.6 details the cost estimate for each piece of equipment as well as raw material and utilities and explains alternative design for economic feasibility.

5.2. Flow Diagram

The process flow diagram (PFD) is attached as a separate file with stream data outlining all pressures, temperatures, flow rates, and compositions along with heat duties and work requirements for each piece of equipment.

5.3. Overall Mass Balances

5.3.1. Reactor 1

	Stream No.	
Component	6	7
Argon	19547	19547
Carbon Dioxide	11824	56578
Di-Ethylene Glycol	0	0
Ethane	10497	10497
Ethylene	950904	855824
Ethylene Glycol	0	0
Ethylene Oxide	19372	146295
Oxygen	357948	263037
Triethylene Glycol	0	0
Water	0	18320
Methane	220364	220364
Amine Solution	0	0
Total	1590455	1590462

Table 20 – Reactor 1 mass balance

5.3.2. EO Desorber & EO Scrubber

	Stream No.			
Component	9	10	47	55
Argon	19547	0	19547	0
Carbon Dioxide	56578	594	55984	0
Di-Ethylene Glycol	0	0	0	0
Ethane	10497	6	10490	0
Ethylene	855824	1377	854447	0
Ethylene Glycol	0	0	0	0
Ethylene Oxide	146295	126746	19571	0

Oxygen	263037	0	263037	0
Triethylene Glycol	0	0	0	0
Water	18320	1178262	19579	1179521
Methane	220364	105	220258	0
Amine Solution	0	0	0	0
Total	1590462	1307091	1462914	1179521

Table 21 – EO Scrubber mass balance

	Stream No.			
Component	11	12	13	57
Argon	0	0	0	0
Carbon Dioxide	594	594	0	0
Di-Ethylene Glycol	0	0	0	0
Ethane	6	6	0	0
Ethylene	1377	1377	0	0
Ethylene Glycol	0	0	0	0
Ethylene Oxide	126746	1560	125186	0
Oxygen	0	0	0	0
Triethylene Glycol	0	0	0	0
Water	1178262	1178262	1075702	1075702
Methane	105	105	0	0
Amine Solution	0	0	0	0
Total	1307091	1181905	1200888	1075702

Table 22- EO Desorber mass balance

5.3.3. CO2 Scrubber

	Stream No.			
Component	51	52	53	56
Argon	19352	19352	0	0
Carbon Dioxide	55424	11825	43337	0
Di-Ethylene Glycol	0	0	0	0
Ethane	10386	10386	0	0
Ethylene	845903	845890	13	0

Ethylene Glycol	0	0	0	0
Ethylene Oxide	19375	19375	0	0
Oxygen	260407	260407	0	0
Triethylene Glycol	0	0	0	0
Water	0	0	0	0
Methane	218056	218056	1	0
Amine Solution	0	0	427980	427980
Total	1428902	1385290	471331	427980

Table 23 – CO2 Scrubber mass balance

5.3.4. Reactor 2

	Stream No.	
Component	16	17
Argon	0	0
Carbon Dioxide	0	0
Di-Ethylene Glycol	0	4713
Ethane	0	0
Ethylene	0	0
Ethylene Glycol	0	170622
Ethylene Oxide	125186	0
Oxygen	0	0
Triethylene Glycol	2	188
Water	1075702	1025358
Methane	0	0
Amine Solution	0	0
Total	1200890	1200881

Table 24 – Reactor 2 mass balance

5.3.5. H_2O Distillation Columns

	Stream No.		
Component	19	23	25
Argon	0	0	0
Carbon Dioxide	0	0	0
Di-Ethylene Glycol	4713	47	4666
Ethane	0	0	0

Ethylene	0	0	0
Ethylene Glycol	170622	171	170452
Ethylene Oxide	0	0	0
Oxygen	0	0	0
Triethylene Glycol	188	2	187
Water	1024489	1014244	10245
Methane	0	0	0
Amine Solution	0	0	0
Total	1200013	1014464	185549

Table 25 – H2O Distillation Column 1 mass balance

	Stream No.		
Component	27	31	34
Argon	0	0	0
Carbon Dioxide	0	0	0
Di-Ethylene Glycol	4666	47	4619
Ethane	0	0	0
Ethylene	0	0	0
Ethylene Glycol	170452	170	170281
Ethylene Oxide	0	0	0
Oxygen	0	0	0
Triethylene Glycol	187	2	185
Water	10245	10157	88
Methane	0	0	0
Amine Solution	0	0	0
Total	185549	10376	175173

Table 26 - H2O Distillation Column 1 mass balance

5.3.6. MEG Distillation Column

	Stream No.		
Component	36	40	44
Argon	0	0	0
Carbon Dioxide	0	0	0
Di-Ethylene Glycol	4619	84	4535
Ethane	0	0	0
Ethylene	0	0	0
Ethylene Glycol	170281	168579	1703
Ethylene Oxide	0	0	0
Oxygen	0	0	0
Triethylene Glycol	185	0	185
Water	88	84	4
Methane	0	0	0
Amine Solution	0	0	0
Total	175173	168747	6426

Table 27 – H2O Distillation Column mass balance

5.3.7. Overall Mass Balance

	Inlet Stream No.						Outlet Stream No.						
Component	1	2	54	56	57	58	12	32	42	46	48	53	60
Argon	0	195	0	0	0	0	0	0	0	0	195	0	0
Carbon Dioxide	0	0	0	0	0	0	594	0	0	0	560	43337	0
Di-Ethylene Glycol	0	0	0	0	0	0	0	94	84	4535	0	0	0
Ethane	105	0	0	0	0	0	6	0	0	0	105	0	0
Ethylene	105044	0	0	0	0	0	1377	0	0	0	8544	13	0
Ethylene Glycol	0	0	0	0	0	0	0	341	168579	1703	0	0	0
Ethylene Oxide	0	0	0	0	0	0	1560	0	0	0	196	0	0
Oxygen	0	97541	0	0	0	0	0	0	0	0	2630	0	0
Triethylene Glycol	0	0	0	0	0	0	0	4	0	185	0	0	0
Water	0	0	1179521	0	1075702	0	1178262	1024401	84	4	196	0	19383
Methane	0	0	0	0	0	2308	105	0	0	0	2203	1	0
Amine Solution	0	0	0	427980	0	0	0	0	0	0	0	427980	0
Total	105150	97736	1179521	427980	1075702	2308	1181905	1024840	168747	6426	14629	471331	19383

Table 28 – Overall Mass Balance by component

Total Mass In [lb/hr]	Total Mass Out [lb/hr]	Difference [lb/hr]	Percent Error
2888396	2887261	1135	0.04%

Table 29 – Total mass input and output

Our overall mass balance had a discrepancy of 1,135 lb/hr or 0.04%. This was considered an acceptable amount of error as we expected some variation in the overall mass balance as we used a variety of different methods to perform calculations. One example of this is using Excel's solver tool, which converges to a value with some level of error. In addition to this, numerical methods such as Euler's method was used to calculate some parts of the process, which can result in a small error.

5.4. Overall Energy Balances

Unit Operations	**Q (MMBtu/hr)**		**W (hp)**	
	Positive (+)	**Negative (-)**	**Positive (+)**	**Negative (-)**
CO2 Scrubber	0.00	0.00	0.00	0.00
EO Descrubber	0.00	0.00	0.00	0.00
EO Scrubber	0.00	0.00	0.00	0.00
H-1	0.0078	-0.0078	0.00	0.00
H-2	0.00	-0.0028	0	0
H-3	0.005	-0.005	0.00	0.00
H-4	0.00	-1346.19	0.00	0.00
H-5	183.67	0.00	0.00	0.00
H-6	0.00	-47.50	0.00	0.00
H-7	0.00	-964.91	0.00	0.00
H-8	819.53	0.00	0.00	0.00
H-9	0.00	-2.54	0.00	0.00
H-10	0.00	-17.34	0.00	0.00
H-11	12.81	0.00	0.00	0.00
H-12	0.00	-13.46	0.00	0.00
H-13	0.00	-89.28	0.00	0.00
H-14	0.00	-18.89	0.00	0.00
H-15	85.07	0.00	0.00	0.00
H-16	0.00	-104.14	0.00	0.00
KO Drum	0.00	0.00	0.00	0.00
MEG Column	0.00	0.00	0.00	0.00
P-1	0.00	0.00	0.00	-148.58
P-2	0.00	0.00	0.00	-179.87
P-3	0.00	0.00	0.00	-1.57
Reactor 1	0.00	-420.08	0.00	0.00
Reactor 2	0.00	-103.20	0.00	0.00
V-1	0.00	0.00	0.00	0.00
V-2	0.00	0.00	0.00	0.00
V-3	0.00	0.00	0.00	0.00
V-4	0.00	0.00	0.00	0.00
V-5	0.00	0.00	0.00	0.00

V-6	0.00	0.00	0.00	0.00
Vent Drum	0.00	0.00	0.00	0.00
C-1	0.00	0.00	0.00	-2224.14

Table 30 – overall energy balances

Total +Q [MMBtu/hr]	Total -Q [MMBtu/hr]	Total Ws [hp]	Total -Ws [hp]
1101.08	-3127.54	0.00	-2554.16

Table 31 – Total cooling and heating duty with total work input

The cooling duty is relatively larger than the heating duty and that is because of the large flowrates and both primary reactions being highly exothermic. This can be combated with more heat integration which is discussed in section 6.3.

5.5. Specifications Sheets

5.5.1. Reactors

Ethylene Epoxidation Reactor				
Identification:	Item:	Reactor	Date:	12/7/20
	Item No:	R-1		
	No. Required:	1		
Function:	React mixture of ethylene with oxygen to produce ethylene oxide			
Operation:	Resident time: 0.005 seconds			
Materials Handled:	Stream No.	6	7	
	Vapor Fraction	1	1	
	Temperature (F)	446	446	
	Pressure (Psig)	275.3	255.3	
	Quantity [lbm/hr]	1590454.9	1590461.7	
Design Data:	Tube material	Stainless Steel		
	Shell material	Stainless Steel		
	Tube diameter [ft]	0.0984		
	Tube length [ft]	32.81		
	No. of tubes	11500		
	Catalyst material	Silver		
	Catalyst shape	Sphere		
Utilities:	Cooling water coming in at 90°F leaving at 120°F			
Comments & Drawings:	Vertical plug flow shell-and-tube reactor (Figure 14) work as a heat exchanger			

Table 32 - Reactor 1 - Specification Sheet

Non-Catalytic Hydrolysis of Ethylene Oxide				
Identification:	Item:	Reactor	Date:	12/7/20
	Item No:	R-2		
	No. Required:	1		
Function:	React ethylene oxide with water to produce ethylene glycol products			
Operation:	Resident time: 2.37 minutes			
Materials Handled:	Stream No.	16	17	
	Vapor Fraction	0	0	
	Temperature (F)	401	401	
	Pressure (Psig)	355.3	355.3	
	Quantity [lbm/hr]	1200889.6	1200881.1	
Design Data:	Tube material	Stainless Steel		
	Shell material	Stainless Steel		
	Tube volume [ft^3]	937.6		
	Tube diameter [ft]	1.9685		
	Tube length [ft]	308.40		
	No. of tubes	1		
Utilities:	Cooling water coming in at 90°F leaving at 120°F			
Comments & Drawings:	work like a heat exchanger (Figure 14) with only 1 tube			

Table 33 - Reactor 2 - Specification Sheet

5.5.2. H2O Distillation Columns

Sieve Tray Column					
Identification:	Item:	*Distillation Column*	Date:		12/7/2020
	Item No:	*H2O Distillation 1*			
	No. Required:	*1*			
Function:	*Separate water from reactor 2 effluent*				
Operation:	*Continuous*				
Materials Handled:	Stream No.	*19*	*23*	*25*	
	Vapor Fraction	*0*	*0*	*0*	
	Temperature (F)	*362.14*	*358.60*	*484.86*	
	Pressure (Psig)	*135.30*	*135.30*	*130.30*	
	Quantity (lb/hr)	*1200012.83*	*1014464.05*	*185548.78*	
Design Data:	Column Diameter (ft)	5.147	No. of trays		*15*
	Column Height (ft)	29.0000	Condenser		*Total*
	Material of Construction	Stainless Steel	Reboiler		*Partial*
	Feed Stage	*14*	Reflux Ratio		*0.1011*
Comments & Drawings:	Figure 7				

Sieve Tray Column					
Identification:	Item:	*Distillation Column*	Date:		12/7/2020
	Item No:	*H2O Distillation 2*			
	No. Required:	*1*			
Function:	*Separate water from Evaporator 1 bottoms outlet*				
Operation:	*Continuous*				
Materials Handled:	Stream No.	*27*	*31*	*35*	
	Vapor Fraction	*0*	*0*	*0*	
	Temperature (F)	*467.62*	*344.91*	*547.33*	
	Pressure (Psig)	*110.30*	*110.30*	*105.30*	
	Quantity (lb/hr)	*185548.78*	*10375.76*	*175173.02*	
Design Data:	Column Diameter (ft)	0.719	No. of trays		*10*
	Column Height (ft)	24.0000	Condenser		*Total*
	Material of Construction	Stainless Steel	Reboiler		*Partial*
	Feed Stage	*8*	Reflux Ratio		*0.9332*
Comments & Drawings:			Figure 7		

Table 34 -H2O Distillation Columns - Specification Sheet

5.5.3. MEG Distillation Column

Sieve Tray Column					
Identification:	Item:	*Distillation Column*	Date:		12/7/2020
	Item No:	*MEG Column*			
	No. Required:	*1*			
Function:	*Separate MEG from Evaporator 2 bottoms outlet*				
Operation:	*Continuous*				
Materials Handled:	Stream No.	*37*	*41*	*45*	
	Vapor Fraction	*0*	*0*	*0*	
	Temperature (F)	*448.71*	*447.66*	*489.82*	
	Pressure (Psig)	*23.03*	*23.03*	*19.03*	
	Quantity (lb/hr)	*175173.02*	*168747.35*	*84261.16*	
Design Data:	Column Diameter (ft)	1.408	No. of trays		*15*
	Column Height (ft)	29.0000	Condenser		*Total*
	Material of Construction	Stainless Steel	Reboiler		*Partial*
	Feed Stage	*13*	Reflux Ratio		*0.5311*
Comments & Drawings:	Figure 7				

Table 35 - MEG Column - Specification Sheet

5.5.4. EO Scrubber

Sieve Tray Column					
Identification :	Item:	*Absorber*	Date:		12/7/2020
	Item No:	*EO Scrubber*			
	No. Required:	*1*			
Function:	*Separate Ethylene Oxide from the reactor effluent stream*				
Operation:	*Continuous*				
Materials Handled:	Stream No.	*9*	*10*	*48*	*56*
	Vapor Fraction	*1*	*0*	*1*	*0*
	Temperature (F)	*447.75*	*95.00*	*447.75*	*95.00*
	Pressure (Psig)	*249.30*	*249.30*	*250.60*	*250.60*
	Quantity (lb/hr)	*1590461.67*	*1307090.65*	*1462913.9*	*1179520.73*
Design Data:	Column Diameter (ft)	17.378	No. of trays		*13*
	Column Height (ft)	58.4544	Actual number of trays		*39*
	Material of Construction	Stainless Steel	Efficiency (%)		*33.24490087*
	Bottom feed Stream	*8*	Top feed Stream		*55*
Comments & Drawings:	Figure 7				

Table 36 - EO Scrubber - Specification Sheet

5.5.5. EO Desorber

Sieve Tray Column					
Identification :	Item:	Stripper	Date:		12/7/2020
	Item No:	EO Desorber			
	No. Required:	1			
Function:	*Separate Ethylene Oxide from the other components that got absorbed with the absorbent*				
Operation:	*Continuous*				
Materials Handled:	Stream No.	*11*	*12*	*13*	*58*
	Vapor Fraction	*0*	*0*	*1*	*1*
	Temperature (F)	*198.92*	*198.92*	*414.00*	*414.00*
	Pressure (Psig)	*242.30*	*247.40*	*277.10*	*275.00*
	Quantity	*1307091*	*1181905*	*1200888*	*1075702*
Design Data:	Column Diameter (ft)	15.11359121	No. of trays		*21*
	Column Height (ft)	86.5288456	Actual number of trays		63.16758195
	Material of Construction	Stainless Steel	Efficiency		*33.24490087*
	Bottom feed Stream	*57*	Top feed Stream		*10*
Comments & Drawings:	Figure 7				

Table 37 - EO Desorber Specification Sheet

1.1.1. CO2 Scrubber

Sieve Tray Column					
Identification :	Item:	Absorber	Date:		12/7/2020
	Item No:	CO2 Scrubber			
	No. Required:	1			
Function:	Separate Carbon Dioxide from the Vent Stream				
Operation:	Continuous				
Materials Handled:	Stream No.	*52*	*53*	*54*	*57*
	Vapor Fraction	*1*	*1*	*0*	*0*
	Temperature (F)	*780.69*	*780.69*	*140.00*	*140.00*
	Pressure (Psig)	*360.90*	*360.00*	*359.10*	*360.00*
	Quantity	*1428902*	*1385290*	*471331*	*427980*
Design Data:	Column Diameter (ft)	22.65600593	No. of trays		*9*
	Column Height (ft)	89.16411208	Actual number of trays		*65.426382*
	Material of Construction	Stainless Steel	Efficiency		*13.755919*
	Bottom feed Stream	*51*	Top feed Stream		*56*
Comments & Drawings:	Figure 7				

Table 38 - CO2 Scrubber Specification Sheet

1.1.2. Pumps

Centrifugal Pump				
Identification :	Item:	*Pump*	Date:	12/7/2020
	Item No:	*P-1*		
	No. Required:	*1*		
Function:	*Increase the pressure of the liquid*			
Operation:	*Continuous*			
Materials Handled:	Stream No.	*14*	*15*	
	Vapor Fraction	*0*	*0*	
	Temperature (F)	*233.00*	*248.91*	
	Pressure (Psig)	*275.60*	*360.30*	
	Quantity (lb/hr)	*1200887.75*	*1200887.75*	
Design Data:	Efficiency (%)	85.000	Head (ft)	*229.5286788*
	Work Shaft (hp)	-148.5848	Volumetric flow rate (gal/min)	*2560*
	Material of Construction	Stainless Steel		
	Input Stream	*14*	Output Stream	*15*
Comments & Drawings:	Figure 1			

Centrifugal Pump				
Identification :	Item:	*Pump*	Date:	12/7/2020
	Item No:	*P-2*		
	No. Required:	*1*		
Function:	*Increase the pressure of the absorbent (water)*			
Operation:	*Continuous*			
Materials Handled:	Stream No.	*55*	*56*	
	Vapor Fraction	*0*	*0*	
	Temperature (F)	*95.00*	*95.00*	
	Pressure (Psig)	*140.00*	*250.60*	
	Quantity (lb/hr)	*1179520.73*	*1179520.73*	
Design Data:	Efficiency (%)	85.000	Head (ft)	*301.5688395*
	Work Shaft (hp)	-179.8657	Volumetric flow rate (gal/min)	*2359.063*
	Material of Construction	Carbon Steel		
	Input Stream	*55*	Output Stream	*56*
Comments & Drawings:	Figure 1			

Centrifugal Pump				
Identification :	Item:	*Pump*	Date:	12/7/2020
	Item No:	*P-3*		
	No. Required:	*1*		
Function:	*Increase the pressure of the liquid*			
Operation:	*Continuous*			
Materials Handled:	Stream No.	*31*	*62*	
	Vapor Fraction	*0*	*0*	
	Temperature (F)	*344.91*	*344.91*	
	Pressure (Psig)	*110.30*	*135.30*	
	Quantity (lb/hr)	*10381.73*	*10381.73*	
Design Data:	Efficiency (%)	85.000	Head (ft)	*283.5073684*
	Work Shaft (hp)	-1.5716	Volumetric flow rate (gal/min)	*22*
	Material of Construction	Iron Casing		
	Input Stream	*31*	Output Stream	*62*
Comments & Drawings:		Figure 1		

Table 39 - Pump Specification Sheet

1.1.3. Compressor

Centrifugal Compressor				
Identification :	Item:	*Compressor*	Date:	12/7/2020
	Item No:	*C-1*		
	No. Required:	*1*		
Function:	*Increase the pressure of the CO2 Scrubber Feed*			
Operation:	*Continuous*			
Materials Handled:	Stream No.	*51*	*52*	
	Vapor Fraction	*1*	*1*	
	Temperature (F)	*239.69*	*508.27*	
	Pressure (Psig)	*248.00*	*360.90*	
	Quantity (lb/hr)	*1428901.67*	*1428901.67*	
Design Data:	Efficiency (%)	85.000	Output Stream	*52*
	Work Shaft (hp)	-2224.1359	Compressor type	Centrifugal
	Material of Construction	Stainless Steel		
	Input Stream	*51*		
Comments & Drawings:		Figure 1		

Table 40 - Compressor Specification Sheet

1.1.4. Heat Exchangers

Heat Exchanger					
Identification :	Item:	Heat Exchanger	Date:		12/7/2020
	Item No:	H-1			
	No. Required:	1			
Function:	Preheat R1 Feed & Cool Reactor Effluent				
Operation:	Continuous				
Materials Handled:	Stream No.	4	5	7	8
	Vapor Fraction	1	1	1	1
	Temperature (F)	261.26	396.00	446.00	320.62
	Pressure (Psig)	281.30	278.30	255.30	252.30
	Quantity [lbm/hr]	1590455	1590454.89	1590461.67	1590461.67
Design Data:	Tube material	SS		Heat Duty [MMBtu/hr]	0.00
	Shell Material	SS			
	Tube Side Stream(s)	4 & 5			
	Shell Side Stream(s)	7 & 8			
Utilities:	N/A				
Comments & Drawings:	Figure 14				

Heat Exchanger					
Identification :	Item:	Heat Exchanger	Date:		12/7/2020
	Item No:	H-2			
	No. Required:	1			
Function:	Preheat R1 Feed				
Operation:	Continuous				
Materials Handled:	Stream No.	5	6		
	Vapor Fraction	1	1		
	Temperature (F)	396.00	446.00		
	Pressure (Psig)	278.30	275.30		
	Quantity [lbm/hr]	1590454.9	1590454.9		
Design Data:	Tube material	SS		Heat Duty [MMBtu/hr]	-0.0027528

	Shell Material	CS			
	Tube Side Stream(s)	5 & 6			
	Shell Side Stream(s)	N/A			
Utilities:	HPS				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger	Date:		12/7/2020
	Item No:	H-3			
	No. Required:	1			
Function:	Preheat EO Scrubber Inlet & Cool EO Scrubber Outlet				
Operation:	Continuous				
Materials Handled:	Stream No.	8	9	10	11
	Vapor Fraction	1	1	1	1
	Temperature (F)	320.62	239.69	95.00	446.00
	Pressure (Psig)	252.30	249.30	249.30	247.40
	Quantity [lbm/hr]	1590461.67	1590461.67	1307090.65	1181904.92
Design Data:	Tube material	SS		Heat Duty [MMBtu/hr]	0.00
	Shell Material	SS			
	Tube Side Stream(s)	8 & 9			
	Shell Side Stream(s)	10 & 11			
Utilities:	N/A				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger	Date:		12/7/2020
	Item No:	H-4			
	No. Required:	1			
Function:	Condense EO Desorber Overhead				
Operation:	Continuous				
Materials Handled:	Stream No.	13	14		
	Vapor Fraction	1	0		

	Temperature (F)	414.00	233.00		
	Pressure (Psig)	277.10	275.60		
	Quantity [lbm/hr]	1200887.75	1200887.75		
Design Data:	Tube material	SS		Heat Duty [MMBtu/hr]	-1346.19
	Shell Material	CS			
	Tube Side Stream(s)	13 & 14			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger	Date:	12/7/2020
	Item No:	H-5		
	No. Required:	1		

Function:	Preheating R2 Feed with evaporated water				
Operation:	Continuous				
Materials Handled:	Stream No.	15	16		
	Vapor Fraction	0	0		
	Temperature (F)	248.91	401.00		
	Pressure (Psig)	360.30	355.30		
	Quantity [lbm/hr]	1200887.75	1200889.63		
Design Data:	Tube material	SS		Heat Duty [MMBtu/hr]	183.67
	Shell Material	CS			
	Tube Side Stream(s)	15 & 16			
	Shell Side Stream(s)	N/A			
Utilities:	HPS				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification:	Item:	Heat Exchanger	Date:	12/7/2020
	Item No:	H-6		
	No. Required:	1		

Function:	Cool Evap 1 Feed				
Operation:	Continuous				
Materials Handled:	Stream No.	18	19		
	Vapor Fraction	0	0		
	Temperature (F)	401.00	362.14		
	Pressure (Psig)	138.30	135.30		
	Quantity [lbm/hr]	1200012.83	1200012.83		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-47.50
	Shell Material	CS			
	Tube Side Stream(s)	18 & 19			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification:	Item:	Heat Exchanger	Date:	12/7/2020	
	Item No:	H-7			
	No. Required:	1			
Function:	Condense Evap 1 Overhead				
Operation:	Continuous				
Materials Handled:	Stream No.	20	21		
	Vapor Fraction	1	0		
	Temperature (F)	358.60	358.60		
	Pressure (Psig)	137.30	135.30		
	Quantity [lbm/hr]	1117012.43	1117012.43		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-964.91
	Shell Material	CS			
	Tube Side Stream(s)	20 & 21			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger		Date:	12/7/2020
	Item No:	H-8			
	No. Required:	1			
Function:	Evap 1 Reboiler				
Operation:	Continuous				
Materials Handled:	Stream No.	24	25		
	Vapor Fraction	0	0		
	Temperature (F)	484.86	484.86		
	Pressure (Psig)	132.30	130.30		
	Quantity [lbm/hr]	1302983.27	185548.78		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	819.53
	Shell Material	CS			
	Tube Side Stream(s)	24 & 25			
	Shell Side Stream(s)	N/A			
Utilities:	HPS				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger		Date:	12/7/2020
	Item No:	H-9			
	No. Required:	1			
Function:	Cool Evap 2 Feed				
Operation:	Continuous				
Materials Handled:	Stream No.	26	27		
	Vapor Fraction	0	0		
	Temperature (F)	484.86	467.62		
	Pressure (Psig)	112.30	110.30		
	Quantity [lbm/hr]	185548.78	185548.78		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-2.54
	Shell Material	CS			
	Tube SideStream(s)	26 & 27			

	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger		Date:	12/7/2020
	Item No:	H-10			
	No. Required:	1			
Function:	Condense Evap 2 Overhead				
Operation:	Continuous				
Materials Handled:	Stream No.	28	29		
	Vapor Fraction	1	0		
	Temperature (F)	344.91	344.91		
	Pressure (Psig)	112.30	112.30		
	Quantity [lbm/hr]	20058.62	20058.62		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-17.34
	Shell Material	CS			
	Tube Side Stream(s)	28 & 29			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger		Date:	12/7/2020
	Item No:	H-11			
	No. Required:	1			
Function:	Evap 2 Reboiler				
Operation:	Continuous				
Materials Handled:	Stream No.	34	35		
	Vapor Fraction	0	0		
	Temperature (F)	547.33	547.33		
	Pressure (Psig)	107.30	105.30		

	Quantity [lbm/hr]	195231.64	175173.02		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	12.81
	Shell Material	CS			
	Tube Side Stream(s)	34 & 35			
	Shell Side Stream(s)	N/A			
Utilities:	HPS				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger		Date:	12/7/2020
	Item No:	H-12			
	No. Required:	1			
Function:	Cool MEG Column Feed				
Operation:	Continuous				
Materials Handled:	Stream No.	36	37		
	Vapor Fraction	0	0		
	Temperature (F)	547.33	448.71		
	Pressure (Psig)	25.03	23.03		
	Quantity [lbm/hr]	175173.02	175173.02		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-13.46
	Shell Material	CS			
	Tube Side Stream(s)	36 & 37			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger	Date:	12/7/2020
	Item No:	H-13		
	No. Required:	1		
Function:	Condense MEG Column Overhead			
Operation:	Continuous			

Materials Handled:	Stream No.	38	39		
	Vapor Fraction	1	0		
	Temperature (F)	447.66	447.66		
	Pressure (Psig)	25.03	23.03		
	Quantity [lbm/hr]	258376.05	258376.05		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-89.28
	Shell Material	CS			
	Tube Side Stream(s)	38 & 39			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger		Date:	12/7/2020
	Item No:	H-14			
	No. Required:	1			
Function:	Cool MEG Product Stream				
Operation:	Continuous				
Materials Handled:	Stream No.	41	42		
	Vapor Fraction	0	0		
	Temperature (F)	447.66	447.66		
	Pressure (Psig)	23.03	20.03		
	Quantity [lbm/hr]	168747.35	92242.74		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-18.89
	Shell Material	CS			
	Tube Side Stream(s)	41 & 42			
	Shell Side Stream(s)	N/A			
Utilities:	CW				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger	Date:		12/7/2020
	Item No:	H-15			
	No. Required:	1			
Function:	MEG Column Reboiler				
Operation:	Continuous				
Materials Handled:	Stream No.	44	45		
	Vapor Fraction	0	0		
	Temperature (F)	489.82	489.82		
	Pressure (Psig)	21.03	19.03		
	Quantity [lbm/hr]	84261.16	84261.16		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	85.07
	Shell Material	CS			
	Tube Side Stream(s)	44 & 45			
	Shell Side Stream(s)	N/A			
Utilities:	HPS				
Comments & Drawings:	Figure 14				

Heat Exchanger

Identification :	Item:	Heat Exchanger	Date:		12/7/2020
	Item No:	H-16			
	No. Required:	1			
Function:	Cool DEG/TEG Product Streams				
Operation:	Continuous				
Materials Handled:	Stream No.	45	46		
	Vapor Fraction	0	0		
	Temperature (F)	489.82	100.00		
	Pressure (Psig)	19.03	17.03		
	Quantity [lbm/hr]	84261.16	84261.16		
Design Data:	Tube material	CS		Heat Duty [MMBtu/hr]	-104.14
	Shell Material	CS			
	Tube Side Stream(s)	45 & 46			
	Shell Side Stream(s)	N/A			

Utilities:	CW
Comments & Drawings:	Figure 14

Table 41 - Heat Exchanger Specification Sheet

5.6. Cost Analysis

5.6.1. Equipment Cost

Table 42 outlines the cost of each piece of equipment with the total equipment cost coming up to $23,467,350. The various methods used to calculate the specific equipment cost are discussed in Section 3.

Figure 17 analyzes the total cost of each type of equipment. Distillation columns are the most expensive, followed by reactors and then the compressor. Distillation columns require multiple stages and trays, so it is plausible for them to be this costly. The total cost of the reactors comes out to be relatively high too, and that is mainly because of the large flow rates as well as reactor 2, having a 99.99% conversion. These two reasons require reactors to have a large volume hence a higher price. The compressor requires work of around 2000 hp which mean has resulted in a high equipment cost.

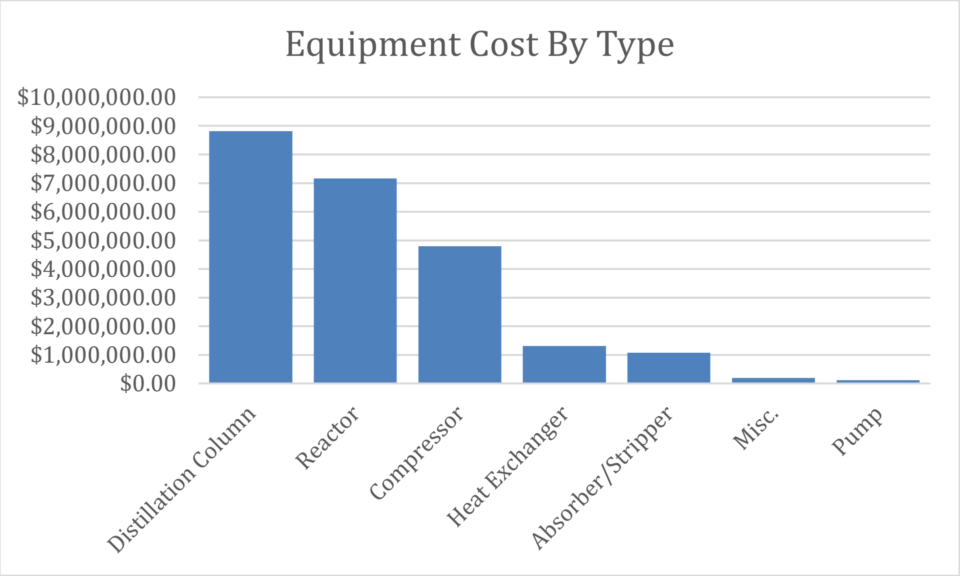


Figure 15 – Equipment Cost by Type

Equipment	Type	Cost ($)
CO2 Scrubber	Absorber/Stripper	$ 743,489.13
Compressor 1	Compressor	$ 4,798,881.45

EO Desorber	Absorber/Stripper	$ 164,904.75
EO Scrubber	Absorber/Stripper	$ 168,138.18
H2O Distillation Column 1	Distillation Column	$ 5,929,152.53
H2O Distillation Column 2	Distillation Column	$ 360,368.52
Heat Exchanger 1	Heat Exchanger	$ 27,641.56
Heat Exchanger 2	Heat Exchanger	$ 15,663.55
Heat Exchanger 3	Heat Exchanger	$ 23,034.63
Heat Exchanger 4	Heat Exchanger	$ 354,485.69
Heat Exchanger 5	Heat Exchanger	$ 208,847.32
Heat Exchanger 6	Heat Exchanger	$ 19,963.35
Heat Exchanger 7	Heat Exchanger	$ 122,851.37
Heat Exchanger 8	Heat Exchanger	$ 293,307.63
Heat Exchanger 9	Heat Exchanger	$ 6,142.57
Heat Exchanger 10	Heat Exchanger	$ 9,213.85
Heat Exchanger 11	Heat Exchanger	$ 10,749.49
Heat Exchanger 12	Heat Exchanger	$ 9,520.98
Heat Exchanger 13	Heat Exchanger	$ 28,409.38
Heat Exchanger 14	Heat Exchanger	$ 30,712.84
Heat Exchanger 15	Heat Exchanger	$ 46,069.26
Heat Exchanger 16	Heat Exchanger	$ 107,494.94
KO Drum	Misc.	$ 39,926.69
MEG Column	Distillation Column	$ 2,522,797.93
Mixer 1	Misc.	$ 39,926.69
Mixer 2	Misc.	$ 39,926.69
Mixer 3	Misc.	$ 9,213.85
Pump 1	Pump	$ 47,604.90
Pump 2	Pump	$ 61,272.12
Pump 3	Pump	$ 3,224.85
Reactor 1	Reactor	$ 5,448,703.74
Reactor 2	Reactor	$ 1,715,206.53
Splitter 1	Misc.	$ 7,524.65
Splitter 2	Misc.	$ 307.13
Splitter 3	Misc.	$ 3,071.28
Valve 1	Misc.	$ 1,612.42
Valve 2	Misc.	$ 1,612.42
Valve 3	Misc.	$ 1,612.42
Valve 4	Misc.	$ 1,612.42
Valve 5	Misc.	$ 1,612.42
Valve 6	Misc.	$ 1,612.42
Vent Drum	Misc.	$ 39,926.69
Total		$ 23,467,350

Table 42 – Process Equipment Costs

5.6.2. Raw Material Costs

Component	Mass Flowrate (lb/hr)	$/hr	$/year
Ethylene	105044.41	$115,857.80	$973,205,550.63
Oxygen	97540.74	$85.56	$718,668.91
Methane	2307.96	$6.84	$57,489.85

Table 43 – Raw Material Costs

5.6.3. Utility Costs

As seen in Figure 18, steam is the predominant utility expense. This result is due to the amount of energy needed to heat boiler feed water to the required specs for MP and HP steam.

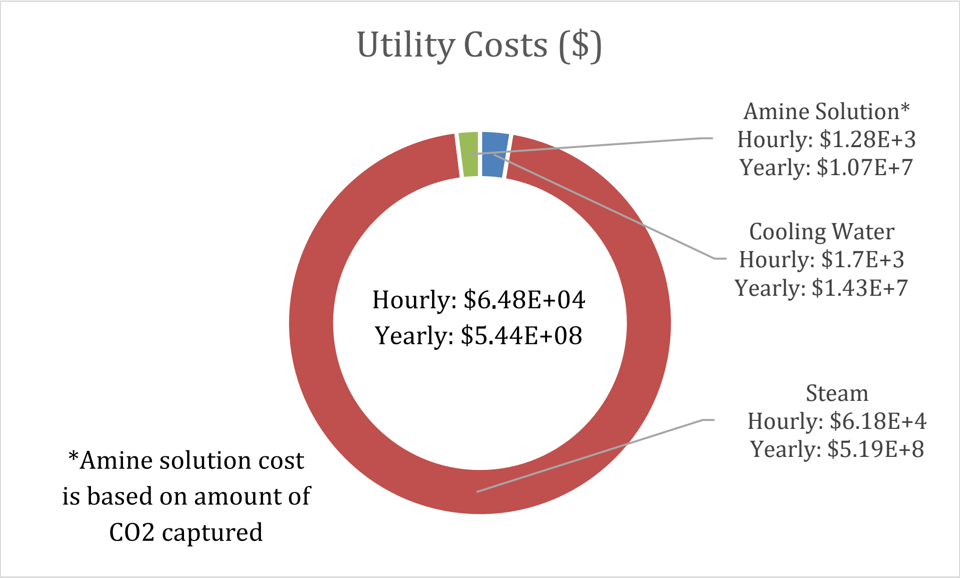


Figure 16 – Utility Cost Chart

Cooling Water Cost			
Equipment	Mass Flowrate (Mlb/hr)	$/hr	$/year
H-6	1586.53	$44.20	$371,316.79
H-7	32229.12	$897.97	$7,542,987.79
H-9	84.90	$2.37	$19,869.94
H-10	579.25	$16.14	$135,569.93
H-12	449.44	$12.52	$105,189.21
H-13	2982.15	$83.09	$697,949.79

H-14	631.00	$17.58	$147,679.79
H-16	3478.46	$96.92	$814,107.72
EO Scrubber	1179.52	$32.86	$276,058.16
Reactor 1	14264.45	$397.44	$3,338,490.44
Reactor 2	3504.21	$97.63	$820,133.82

Steam Cost			
Equipment	Mass Flowrate (Mlb/hr)	$1000/hr	$1000/year
H-5	1559.46	$14.11	$118,542.85
H-8	5269.79	$47.69	$400,584.09
H-11	82.37	$0.75	$6,261.36
H-15	547.03	$4.95	$41,582.50
EO Desorber	1075.70	$8.45	$70,956.09

Amine (MEA) Solution Cost			
Equipment	CO2 Captured (Mlb/hr)	$1000/hr	$1000/year
CO2 Scrubber	43.34	$1.28	$10,716.57

Table 44 - Utility Costs

5.6.4. Cost Estimation Sheet

Cost Estimation Sheet		
	%	Calculated
Direct Costs (Inside Battery limits)		
Purchased Equipment	1	$ 23,467,351.3
Delivery, fraction of purchased	0.1	$ 2,346,735.1
Subtotal: Delivered Equipment		**$ 25,814,086.4**
Purchased Equipment Installation	0.47	$ 12,132,620.6
Instrumentation & Controls (installed)	0.36	$ 9,293,071.1
Piping (installed)	0.68	$ 17,553,578.8
Electrical Systems (installed)	0.11	$ 2,839,549.5
Buildings (including services)	0.18	$ 4,646,535.6
Yard Improvements	0.1	$ 2,581,408.6
Service Facilities (installed)	0.7	$ 18,069,860.5
Total ISBL		**$ 92,930,711.1**
Outside Battery limits (OBSL)	0.3	**$ 27,879,213.3**
Fixed Capital Investment (FCI)		**$ 120,809,924.4**
Contingency	0.2	**$ 48,323,800.0**
Working Capital (WC)	0.3	**$ 72,485,700.0**

Total Capital Investment (TCI)	**$ 241,619,000.00**

Table 45 – Cost Estimation Sheet

5.6.5. Comparison of economics for CO_2 processing

Based on our current projections of carbon dioxide production and the current cost of carbon dioxide processing to remove CO2 from our CO2 scrubber liquid outlet stream, we can approximate the additional cost of the offsite processing to be between $12.5 and $18.2 million /yr [36]. This cost could be reduced by potentially designing additional separation units within the current design that would have the capability of removing the CO_2 in-house with an approximated cost of $1 million for a CO_2 desorbing column, with additional operating expenses associated with the stripping of CO_2 from our MEA solution. This has the potential to reduce our operating cost of the CO_2 absorption column as well by recycling the MEA in our CO_2 removal system. The additional savings by the recovery of this absorbing liquid along with specific costs of additional auxiliary equipment will be calculated to determine the best path forward regarding this.

6. Recommendations

6.1. Fresh Water Conservation

Freshwater is being used as an absorbent, stripping stream, and well as for Reactor 2. To combat this problem, one design change made is that the water from the EO Desorber will be sent to Reactor 2 so that freshwater is not being fed in. However, there is still a huge amount of water fed into the EO Scrubber and water exiting through the H2O Distillation column. A future optimization would be to design a system where the water exiting the distillation columns can be used as the absorbent.

6.2. Separation of DEG & TEG

More distillation columns will be needed to be added downstream for further separation of DEG & TEG. This will allow us to sell DEG & TEG as separate products and will be a profitable addition. This will be an option that will be explored after doing a cost-benefit analysis.

6.3. Heat Integration

Currently, 14 of 16 of our heat exchangers are being heated or cooled with utilities. We plan on taking advantage of this later in the Spring semester, using heat from certain process streams to heat colder process streams. This will allow us to reduce both our total heating and cooling duties required to operate our plant.

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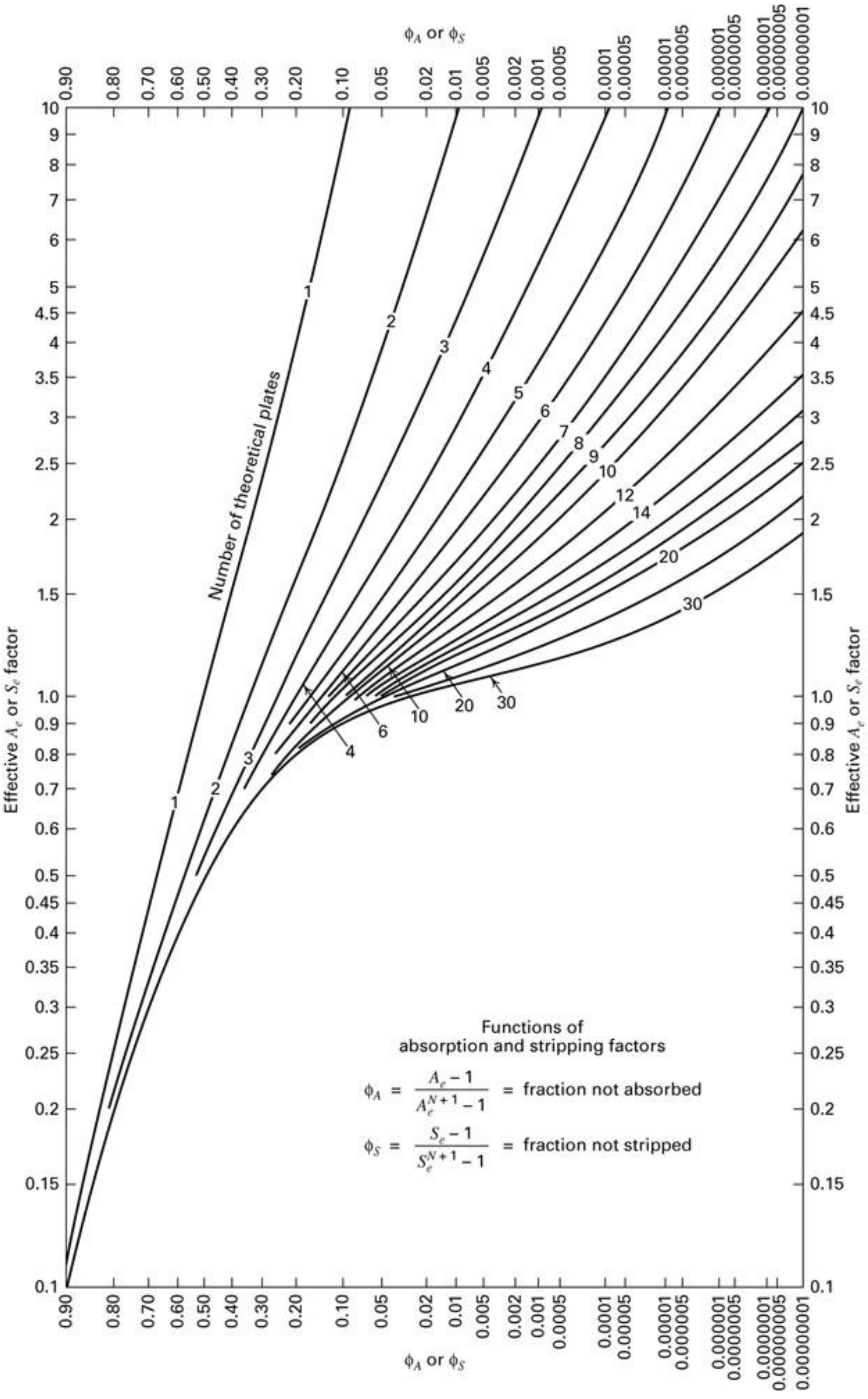
Appendix I – Kremser plot



Appendix II - Calculations

1. Vapor Pressure

1.1. Antoine Equation:

$$\ln P^{sat}\,(bar) = A - \frac{B}{T(K) + C}$$

- Using the coefficients (A, B & C) found in the reference textbook, Thermodynamics Fundamentals and Application for Chemical Engineers pg 439 - 440, the vapor pressure at a given temperature can be calculated using the above-stated equation.
- This equation was used to determine the phase of the components.

2. Heat Capacity

$$\frac{C_P}{R} = A + BT + CT^2 + DT^{-2} + ET^3 \; with\; T\; in\; K\; and\; C_p\; in\; \frac{KJ}{mol}$$

$$R = 8.314 \times 10^{-3}\,\frac{KJ}{mol\,K}$$

- Using the coefficients found in the reference textbook Fleischer pg 440 - 443, the heat capacity of a component at a given temperature can be calculated using the above-stated equation.
- This equation was used to determine the enthalpies for energy balances.

3. Ethylene Epoxidation Reactor Calculation

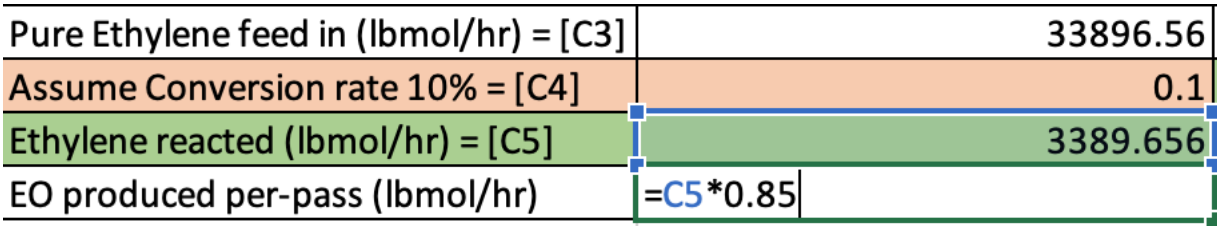
3.1. Reaction equations

$$A + \frac{1}{2}B \rightarrow C$$

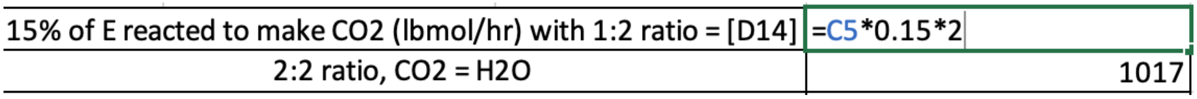
$$A + 3B \rightarrow 2D + 2E$$

$$C + \frac{5}{2}B \rightarrow 2D + 2E$$

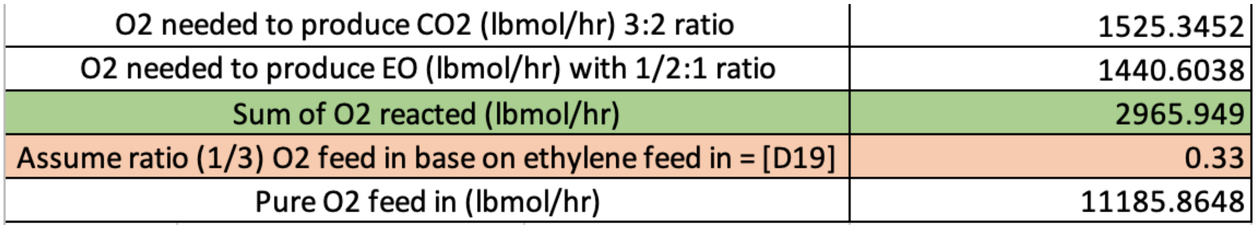
3.2. Mass Balance Calculation



Pure Ethylene feed in (lbmol/hr) = [C3]	33896.56
Assume Conversion rate 10% = [C4]	0.1
Ethylene reacted (lbmol/hr) = [C5]	3389.656
EO produced per-pass (lbmol/hr)	=C5*0.85

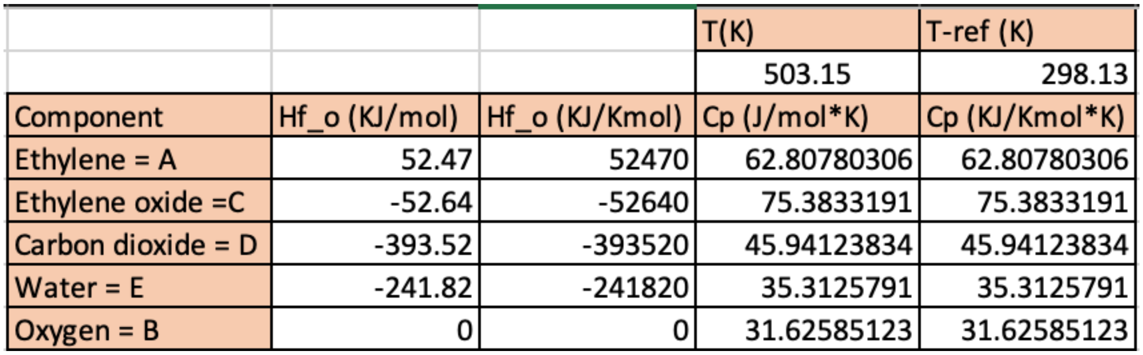


15% of E reacted to make CO2 (lbmol/hr) with 1:2 ratio = [D14]	=C5*0.15*2
2:2 ratio, CO2 = H2O	1017



O2 needed to produce CO2 (lbmol/hr) 3:2 ratio	1525.3452
O2 needed to produce EO (lbmol/hr) with 1/2:1 ratio	1440.6038
Sum of O2 reacted (lbmol/hr)	2965.949
Assume ratio (1/3) O2 feed in base on ethylene feed in = [D19]	0.33
Pure O2 feed in (lbmol/hr)	11185.8648

3.3. Energy Balance Calculation



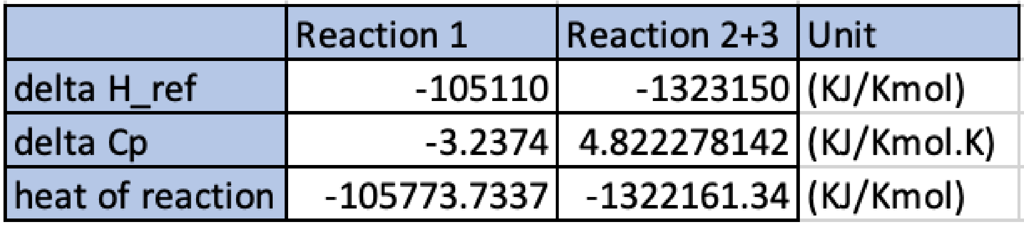
			T(K)	T-ref (K)
			503.15	298.13
Component	Hf_o (KJ/mol)	Hf_o (KJ/Kmol)	Cp (J/mol*K)	Cp (KJ/Kmol*K)
Ethylene = A	52.47	52470	62.80780306	62.80780306
Ethylene oxide =C	-52.64	-52640	75.3833191	75.3833191
Carbon dioxide = D	-393.52	-393520	45.94123834	45.94123834
Water = E	-241.82	-241820	35.3125791	35.3125791
Oxygen = B	0	0	31.62585123	31.62585123

$$\Delta H_{Rx2} = \Delta H_{Rx3}$$

$$\Delta H_{Rx1} = H_C^o - \left(\frac{1}{2}\right) H_B^o - H_A^o + \left[\left(C_{PC} - \left(\frac{1}{2}\right) C_{PB} - C_{PA}\right) * (T - T_R)\right]$$

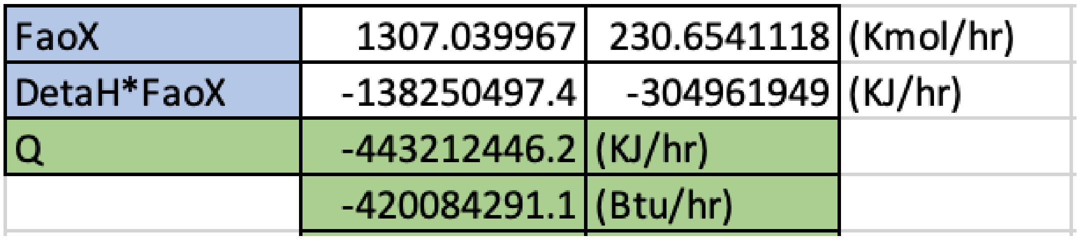
$$\Delta H_{Rx2} = 2H_D^o + 2H_E^o - 3H_B^o - H_A^o + [(2C_{PD} + 2C_{PE} - 3C_{PB} - C_{PA}) * (T - T_R)]$$

T_R = 76.73°F



	Reaction 1	Reaction 2+3	Unit
delta H_ref	-105110	-1323150	(KJ/Kmol)
delta Cp	-3.2374	4.822278142	(KJ/Kmol.K)
heat of reaction	-105773.7337	-1322161.34	(KJ/Kmol)

$$\dot{Q} = \Delta H_{Rx1} F_{Ao} X_{A1} + \Delta H_{Rx2} F_{Ao} X_{A2} + \Delta H_{Rx3} F_C X_C$$



FaoX	1307.039967	230.6541118	(Kmol/hr)
DetaH*FaoX	-138250497.4	-304961949	(KJ/hr)
Q	-443212446.2	(KJ/hr)	
	-420084291.1	(Btu/hr)	

4. Separation of Ethylene Oxide & CO_2 Capture for Ethylene Recovery

4.1. Definitions

4.1.1. $Y_N = (\frac{y}{1-y})_N$

4.1.2. $X_N = (\frac{x}{1-x})_N$

4.1.3. $V_N = V'Y_N$

4.1.4. $L_N = L'X_N$

4.1.5. Absorption factor: $A = \frac{L'}{V'}\frac{1}{K}$

4.1.6. Stripping Factor: $S = \frac{V'}{L'}K$

4.1.7. $X_1 = \frac{Y_1}{Y_1(K_1-1)+K_1}$

4.2. Calculations

4.2.1. EO Scrubber

Absorption equilibrium of solute A, K_A	1.30
L'/V'	1.18
Number of stages, N	13
Solute-free Vapor V'	55605.15
Solute-free Liquid L'	65473.86
x_0 = fresh water	0
y_{N+1} = Reactor Effluent	0.05972
y_1 = purge	0.00799

	Stage	X_A^N	Y_A^N	L_A^N	V_A^N
Feed Liquid	0	0		0.00	
Prod Vapor	1	0.00612	0.00799	400.97	444.26
	2	0.01163	0.01520	761.60	845.24
	3	0.01657	0.02169	1084.92	1205.87
	4	0.02099	0.02750	1373.97	1529.19
	5	0.02492	0.03270	1631.73	1818.24
	6	0.02842	0.03733	1861.05	2075.99
	7	0.03153	0.04146	2064.68	2305.32
	8	0.03429	0.04512	2245.16	2508.94
	9	0.03673	0.04837	2404.87	2689.42
	10	0.03889	0.05124	2546.01	2849.13
	11	0.04079	0.05378	2670.57	2990.27
	12	0.04247	0.05602	2780.39	3114.84
Prod Liquid, LN	13	0.04394	0.05799	2877.12	3224.66
Feed Vap (N+1)	14		0.05973		3321.38
	Stage N+1 Target		0.05972		3320.88
Error:	Compare calc V_A^{N+1} with target V_A^{N+1}				2.52E-01

Check Material Balance:

Flow of A in, $V_A^{N+1} + L_A^0$	3320.882
Flow of A out, $V_A^1 + L_A^N$	3321.385

4.2.2. EO Desorber

Stripping equilibrium of solute A, K_A	1.21
V'/L'	0.91
Number of stages, N	7
Solute-free Vapor V'	59711.46391
Solute-free Liquid L'	65473.86499
x_0	0.04394
y_{N+1}	0.00000
y_1	0.04759

	Stage	X_A^N	Y_A^N	L_A^N	V_A^N
Feed Liquid	0	0.044	0.000	2877.122	0.000
Prod Vapor	1	0.039	0.048	2548.300	2841.707
	2	0.034	0.042	2255.588	2512.885
	3	0.030	0.037	1994.550	2220.174
	4	0.027	0.033	1761.381	1959.135
	5	0.024	0.029	1552.805	1725.966
	6	0.021	0.025	1365.987	1517.390
	7	0.018	0.022	1198.465	1330.573
	8	0.016	0.019	1048.088	1163.050
	9	0.014	0.017	912.978	1012.673

	10	0.012	0.015	791.481	877.563
	11	0.010	0.013	682.146	756.067
	12	0.009	0.011	583.687	646.731
	13	0.008	0.009	494.969	548.272
	14	0.006	0.008	414.984	459.554
	15	0.005	0.006	342.837	379.569
	16	0.004	0.005	277.730	307.422
	17	0.003	0.004	218.954	242.315
	18	0.003	0.003	165.873	183.539
	19	0.002	0.002	117.919	130.458
	20	0.001	0.001	74.585	82.504
Prod Liquid, LN	21	0.001	0.001	35.415	39.170
Feed Vap (N+1)	22	0.000	0.000	0.000	0.000
	Stage N+1 Target		0.000		0.000
Error:	Compare calc V_A^{N+1} with target V_A^{N+1}				0.00000000000

Check Material Balance:

Flow of A in, $V_A^{N+1} + L_A^0$	2877.122
Flow of A out, $V_A^1 + L_A^N$	2877.122

4.2.3. CO_2 Scrubber

Absorption equilibrium of solute A, K_A	0.18
L'/V'	0.13
Number of stages, N	9
Solute-free Vapor V'	53154.13
Solute-free Liquid L'	7006.87
x_0 = (amine absorbing liquid)	0
y_{N+1} = from the vent	0.02369
y_1 = recycle	0.00505

Stage	X_A^N	Y_A^N	L_A^N	V_A^N
0	0		0.00	
1	0.02906	0.00505	203.64	268.68
2	0.05203	0.00889	364.57	472.32
3	0.07079	0.01191	496.03	633.26
4	0.08653	0.01439	606.32	764.71
5	0.10004	0.01646	700.95	875.00
6	0.11185	0.01824	783.73	969.63
7	0.12236	0.01980	857.37	1052.41

8	0.13185	0.02118	923.86	1126.05
9	0.14053	0.02244	984.71	1192.54
10		0.02358		1253.39
Stage N+1 Target		0.02369		1259.34
Compare calc V_A^{N+1} with target V_A^{N+1}				3.54E+01

Check Material Balance:

Flow of A in, $V_A^{N+1} + L_A^0$	1259.344
Flow of A out, $V_A^1 + L_A^N$	1253.394

5. Ethylene Glycol Reactor

5.1. Reaction equations

$$A + B \rightarrow C$$
$$A + C \rightarrow D$$
$$A + D \rightarrow E$$

5.2. Mass Balance Calculation

$$k = A * exp\left[-\frac{E_A}{RT}\right]$$

R (KJ/Kmol.K)	8.314			
Reaction	Ao (m3/kmol-s)	Ea(KJ/Kmol)	k (m3/kmol.s)	rate (kmol/m3.s)
1	5.30E+05	78000	0.001595871	k[EO][H2O]
2	1.00E+06	82000	0.001100863	k[EO][MEG]
3	2.00E+06	81000	0.002831461	k[EO][DEG]

$$\frac{dF_A}{dV} = r_A$$
$$\frac{dC_A}{dV} = \frac{r_A}{v_o}$$
$$dC_A = \frac{r_A}{v_o} * dV$$

$$C_{A(n+1)} = \frac{r_{An}}{v_o} * dV + C_{An}$$ for n = 0,1,2…

With: $r_{An} = -k_1 C_{An} C_{Bn} - k_2 C_{An} C_{Cn} - k_3 C_{An} C_{Bn}$

dV = 0.05 (ft^3)

and at: $V_o = 0$, $C_A = C_{Ao}$

$$C_{A1} = \left(\frac{-k_1 C_{Ao} C_{Bo} - k_2 C_{Ao} C_{Co} - k_3 C_{Ao} C_{Do}}{v_o}\right) * dV + C_{Ao}$$

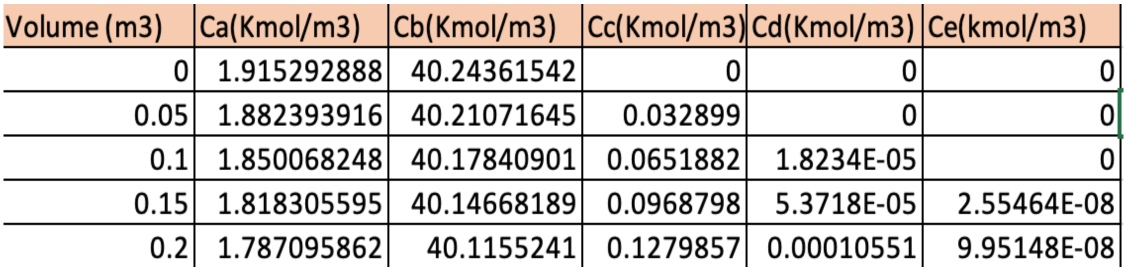
$$C_{B1} = \left(\frac{-k_1 C_{Ao} C_{Bo}}{v_o}\right) * dV + C_{Bo}$$

$$C_{C1} = \left(\frac{k_1 C_{Ao} C_{Bo} - k_2 C_{Ao} C_{Co}}{v_o}\right) * dV + C_{Co}$$

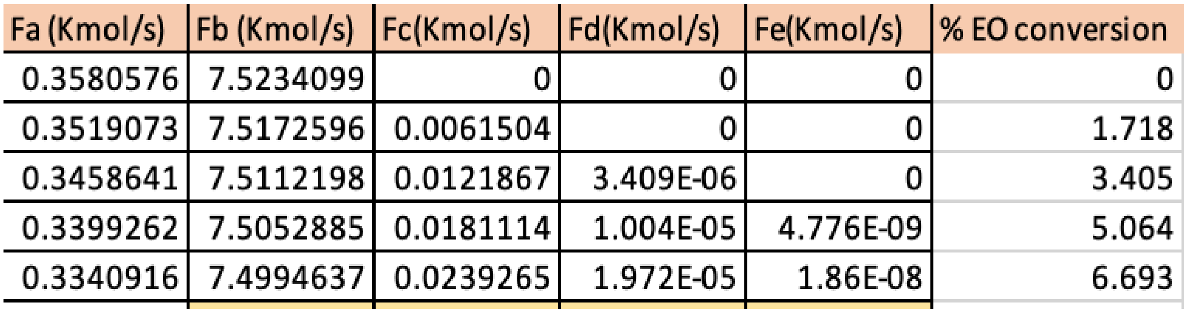
$$C_{D1} = \left(\frac{k_2 C_{Ao} C_{Co} - k_3 C_{Ao} C_{Do}}{v_o}\right) * dV + C_{Do}$$

$$C_{E1} = \left(\frac{k_3 C_{Ao} C_{Do}}{v_o}\right) * dV + C_{Eo}$$

The first 5 steps using the Euler method

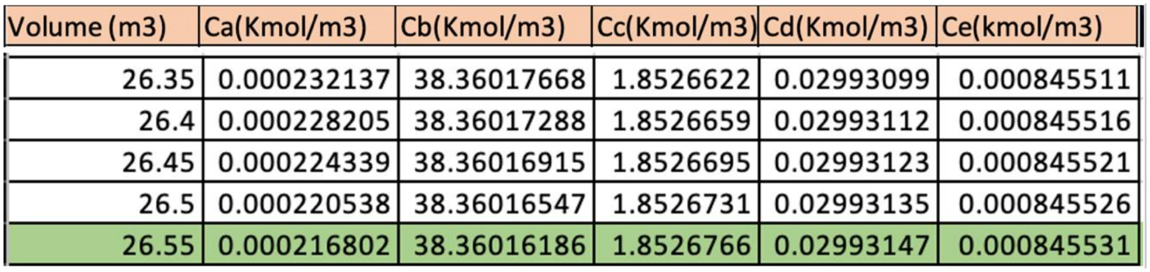


Volume (m3)	Ca(Kmol/m3)	Cb(Kmol/m3)	Cc(Kmol/m3)	Cd(Kmol/m3)	Ce(kmol/m3)
0	1.915292888	40.24361542	0	0	0
0.05	1.882393916	40.21071645	0.032899	0	0
0.1	1.850068248	40.17840901	0.0651882	1.8234E-05	0
0.15	1.818305595	40.14668189	0.0968798	5.3718E-05	2.55464E-08
0.2	1.787095862	40.1155241	0.1279857	0.00010551	9.95148E-08

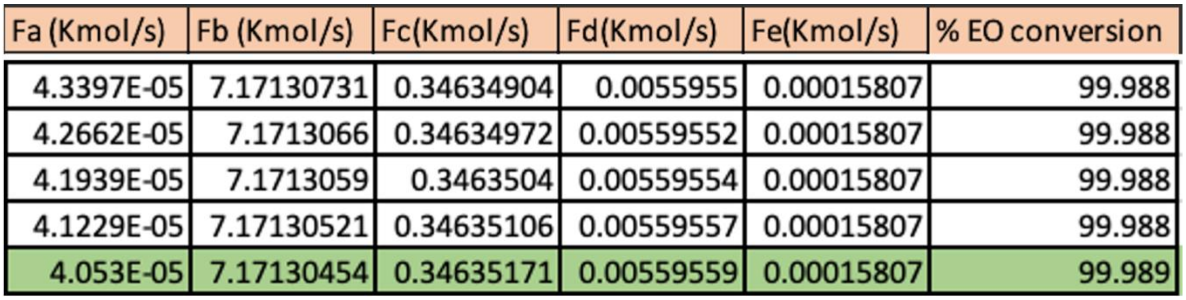


Fa (Kmol/s)	Fb (Kmol/s)	Fc(Kmol/s)	Fd(Kmol/s)	Fe(Kmol/s)	% EO conversion
0.3580576	7.5234099	0	0	0	0
0.3519073	7.5172596	0.0061504	0	0	1.718
0.3458641	7.5112198	0.0121867	3.409E-06	0	3.405
0.3399262	7.5052885	0.0181114	1.004E-05	4.776E-09	5.064
0.3340916	7.4994637	0.0239265	1.972E-05	1.86E-08	6.693

The last 5 steps using the Euler method



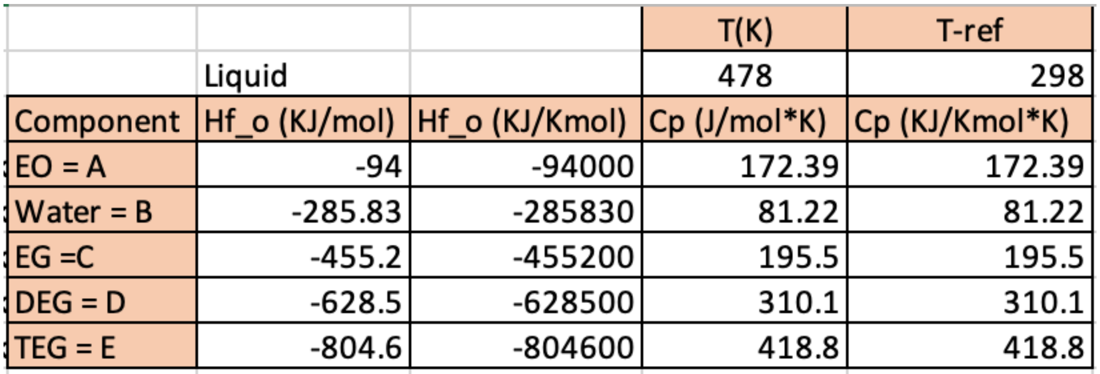
Volume (m3)	Ca(Kmol/m3)	Cb(Kmol/m3)	Cc(Kmol/m3)	Cd(Kmol/m3)	Ce(kmol/m3)
26.35	0.000232137	38.36017668	1.8526622	0.02993099	0.000845511
26.4	0.000228205	38.36017288	1.8526659	0.02993112	0.000845516
26.45	0.000224339	38.36016915	1.8526695	0.02993123	0.000845521
26.5	0.000220538	38.36016547	1.8526731	0.02993135	0.000845526
26.55	0.000216802	38.36016186	1.8526766	0.02993147	0.000845531



Fa (Kmol/s)	Fb (Kmol/s)	Fc(Kmol/s)	Fd(Kmol/s)	Fe(Kmol/s)	% EO conversion
4.3397E-05	7.17130731	0.34634904	0.0055955	0.00015807	99.988
4.2662E-05	7.1713066	0.34634972	0.00559552	0.00015807	99.988
4.1939E-05	7.1713059	0.3463504	0.00559554	0.00015807	99.988
4.1229E-05	7.17130521	0.34635106	0.00559557	0.00015807	99.988
4.053E-05	7.17130454	0.34635171	0.00559559	0.00015807	99.989

The last step is to convert all of the molar flow rates to mass flow rates.

5.3. Energy Balance

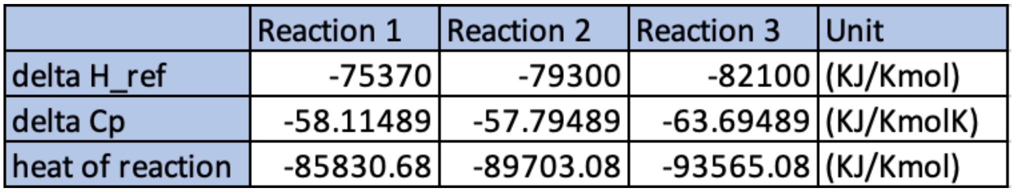


			T(K)	T-ref
	Liquid		478	298
Component	Hf_o (KJ/mol)	Hf_o (KJ/Kmol)	Cp (J/mol*K)	Cp (KJ/Kmol*K)
EO = A	-94	-94000	172.39	172.39
Water = B	-285.83	-285830	81.22	81.22
EG =C	-455.2	-455200	195.5	195.5
DEG = D	-628.5	-628500	310.1	310.1
TEG = E	-804.6	-804600	418.8	418.8

$$\Delta H_{Rx1} = H_C^o - H_B^o - H_A^o + [(C_{PC} - C_{PB} - C_{PA}) * (T - T_R)]$$

$$\Delta H_{Rx2} = H_D^o - H_C^o - H_A^o + [(C_{PD} - C_{PC} - C_{PA}) * (T - T_R)]$$

$$\Delta H_{Rx3} = H_E^o - H_D^o - H_A^o + [(C_{PE} - C_{PD} - C_{PA}) * (T - T_R)]$$

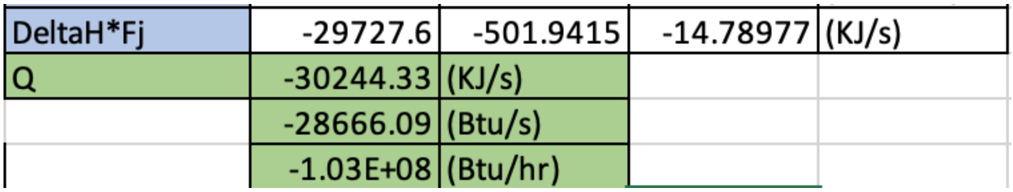


	Reaction 1	Reaction 2	Reaction 3	Unit
delta H_ref	-75370	-79300	-82100	(KJ/Kmol)
delta Cp	-58.11489	-57.79489	-63.69489	(KJ/KmolK)
heat of reaction	-85830.68	-89703.08	-93565.08	(KJ/Kmol)

$$\dot{Q} = \Delta H_{Rx1} F_{Ao} X + \Delta H_{Rx2} F_{Co} X + \Delta H_{Rx3} F_{Do} X$$

$$F_{Ao} X_A = F_C \qquad F_{Co} X_C = F_D \qquad F_{Do} X_D = F_E$$

$$\dot{Q} = \Delta H_{Rx1} F_C + \Delta H_{Rx2} F_D + \Delta H_{Rx3} F_E$$



DeltaH*Fj	-29727.6	-501.9415	-14.78977	(KJ/s)
Q	-30244.33	(KJ/s)		
	-28666.09	(Btu/s)		
	-1.03E+08	(Btu/hr)		

6. H2O Distillation Column

Definitions:

Overall material balance

$$F = D + B$$

Component flow rates

$$f_i = F x_{Fi}$$
$$b_i = B x_{Bi}$$
$$d_i = D x_{Di}$$

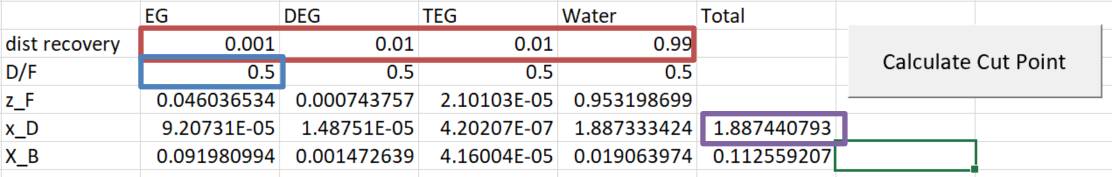
Cut point

$$\frac{D}{F}$$

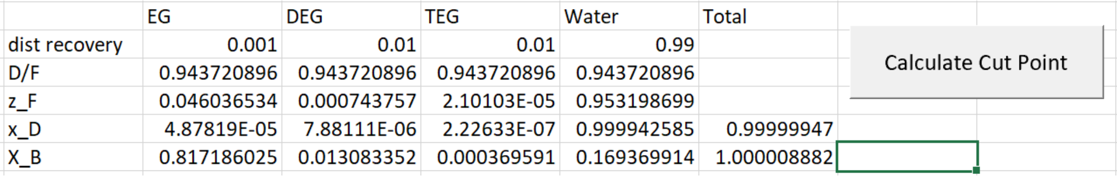
Distillate recovery

$$\frac{d_i}{f_i} = \frac{x_{Di} D}{x_{Fi} F}$$

First, the cut point was determined using Excel Solver. The screenshot below shows the set-up for doing this. The row in the red box contains the distillate recoveries which are the main inputs. Once they were set, the button to the right was pressed to launch Solver. The cell in blue was manipulated until the cell in the purple box equaled 1 or as close to 1 as possible.

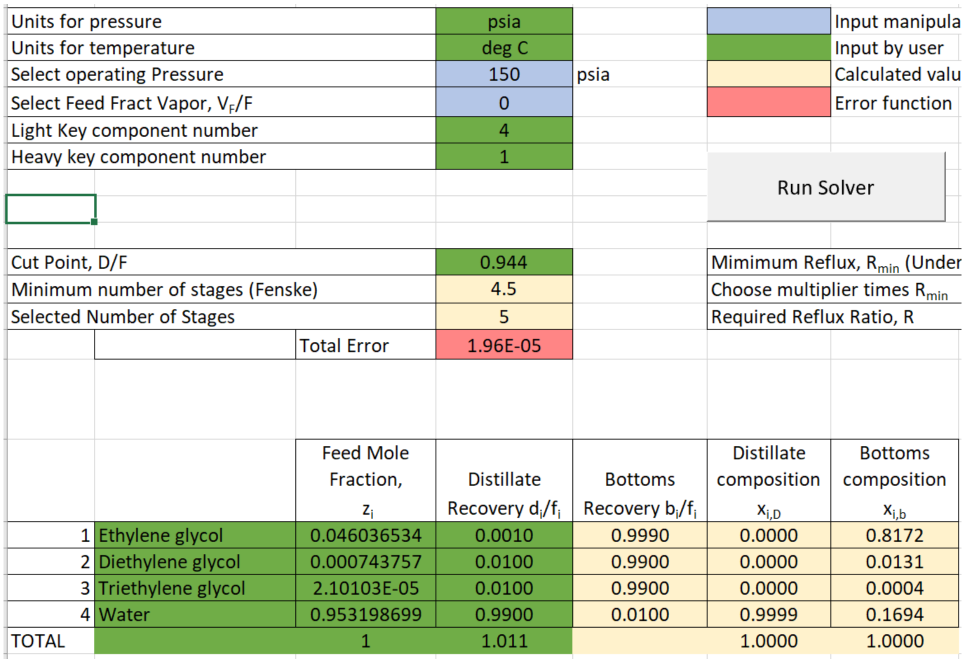


	EG	DEG	TEG	Water	Total
dist recovery	0.001	0.01	0.01	0.99	
D/F	0.5	0.5	0.5	0.5	
z_F	0.046036534	0.000743757	2.10103E-05	0.953198699	
x_D	9.20731E-05	1.48751E-05	4.20207E-07	1.887333424	1.887440793
X_B	0.091980994	0.001472639	4.16004E-05	0.019063974	0.112559207



	EG	DEG	TEG	Water	Total
dist recovery	0.001	0.01	0.01	0.99	
D/F	0.943720896	0.943720896	0.943720896	0.943720896	
z_F	0.046036534	0.000743757	2.10103E-05	0.953198699	
x_D	4.87819E-05	7.88111E-06	2.22633E-07	0.999942585	0.99999947
X_B	0.817186025	0.013083352	0.000369591	0.169369914	1.000008882

With the cut point, distillate recoveries, and distillate compositions determined, values for the column's operating pressure and feed vapor fraction were chosen. In the case of H2O Distillation Column 1, we assumed an operating pressure of 150 psia and feed vapor fraction of 0. We picked the pressure value to allow for flexibility of determining pressures for downstream columns and the feed vapor fraction does not have to introduce more heat exchangers to vaporize the feed stream.

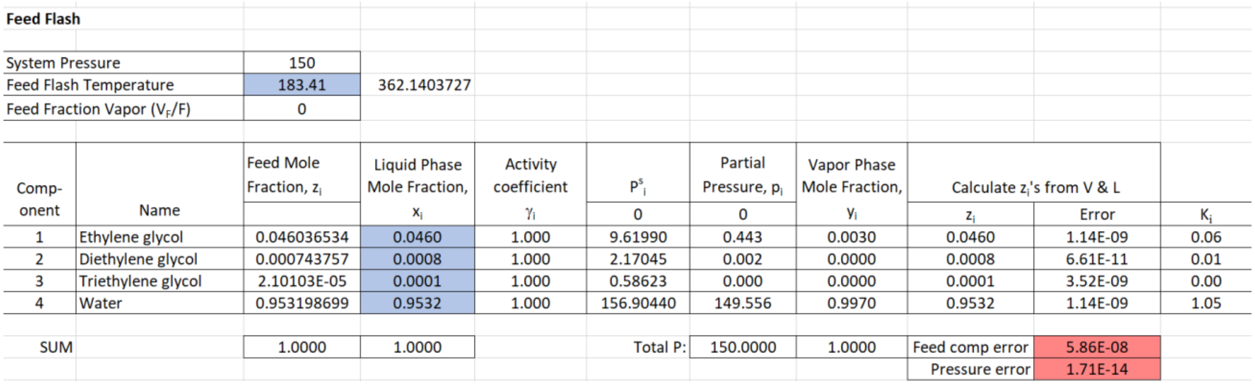


Units for pressure	psia		🟦	Input manipula
Units for temperature	deg C		🟩	Input by user
Select operating Pressure	150	psia	🟨	Calculated valu
Select Feed Fract Vapor, V_F/F	0		🟥	Error function
Light Key component number	4			
Heavy key component number	1			

Cut Point, D/F	0.944	Mimimum Reflux, R_{min} (Under
Minimum number of stages (Fenske)	4.5	Choose multiplier times R_{min}
Selected Number of Stages	5	Required Reflux Ratio, R
Total Error	1.96E-05	

		Feed Mole Fraction, z_i	Distillate Recovery d_i/f_i	Bottoms Recovery b_i/f_i	Distillate composition $x_{i,D}$	Bottoms composition $x_{i,b}$
1	Ethylene glycol	0.046036534	0.0010	0.9990	0.0000	0.8172
2	Diethylene glycol	0.000743757	0.0100	0.9900	0.0000	0.0131
3	Triethylene glycol	2.10103E-05	0.0100	0.9900	0.0000	0.0004
4	Water	0.953198699	0.9900	0.0100	0.9999	0.1694
TOTAL		1	1.011		1.0000	1.0000

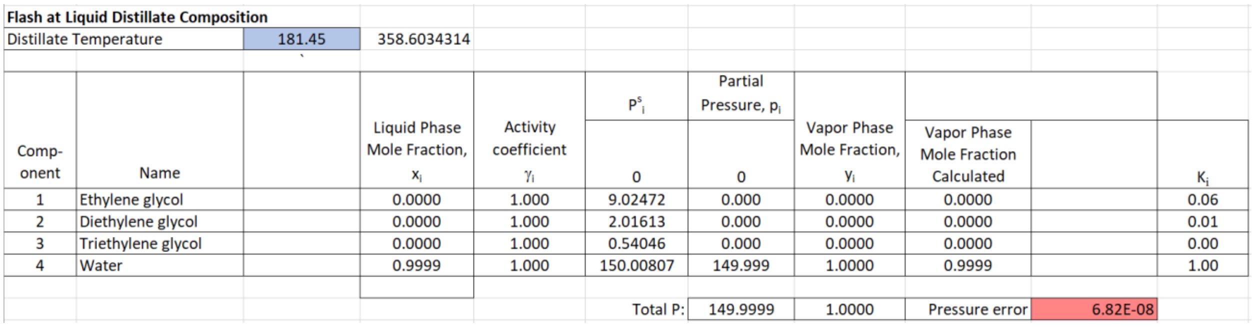
When we pressed the "Run Solver" button, the feed flash liquid compositions and flash temperatures of the feed, distillate, and bottoms were manipulated until the "Total Error" cell reached a minimum value.



Feed Flash

System Pressure	150	
Feed Flash Temperature	183.41	362.1403727
Feed Fraction Vapor (V_F/F)	0	

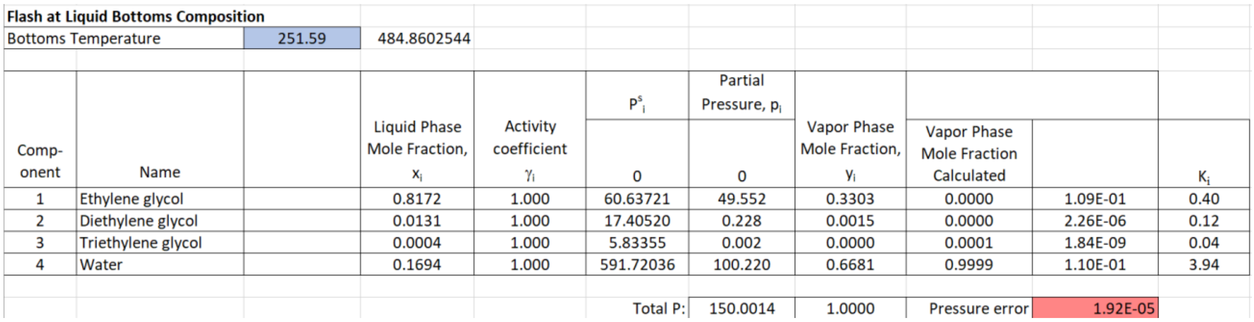
Comp-onent	Name	Feed Mole Fraction, z_i	Liquid Phase Mole Fraction, x_i	Activity coefficient γ_i	P^s_i 0	Partial Pressure, p_i 0	Vapor Phase Mole Fraction, y_i	Calculate z_i's from V & L z_i	Error	K_i
1	Ethylene glycol	0.046036534	0.0460	1.000	9.61990	0.443	0.0030	0.0460	1.14E-09	0.06
2	Diethylene glycol	0.000743757	0.0008	1.000	2.17045	0.002	0.0000	0.0008	6.61E-11	0.01
3	Triethylene glycol	2.10103E-05	0.0001	1.000	0.58623	0.000	0.0000	0.0001	3.52E-09	0.00
4	Water	0.953198699	0.9532	1.000	156.90440	149.556	0.9970	0.9532	1.14E-09	1.05
SUM		1.0000	1.0000		Total P:	150.0000	1.0000	Feed comp error	5.86E-08	
								Pressure error	1.71E-14	



Flash at Liquid Distillate Composition

Distillate Temperature	181.45	358.6034314

Comp-onent	Name		Liquid Phase Mole Fraction, x_i	Activity coefficient γ_i	P^s_i 0	Partial Pressure, p_i 0	Vapor Phase Mole Fraction, y_i	Vapor Phase Mole Fraction Calculated		K_i
1	Ethylene glycol		0.0000	1.000	9.02472	0.000	0.0000	0.0000		0.06
2	Diethylene glycol		0.0000	1.000	2.01613	0.000	0.0000	0.0000		0.01
3	Triethylene glycol		0.0000	1.000	0.54046	0.000	0.0000	0.0000		0.00
4	Water		0.9999	1.000	150.00807	149.999	1.0000	0.9999		1.00
					Total P:	149.9999	1.0000	Pressure error	6.82E-08	



Flash at Liquid Bottoms Composition

Bottoms Temperature	251.59	484.8602544

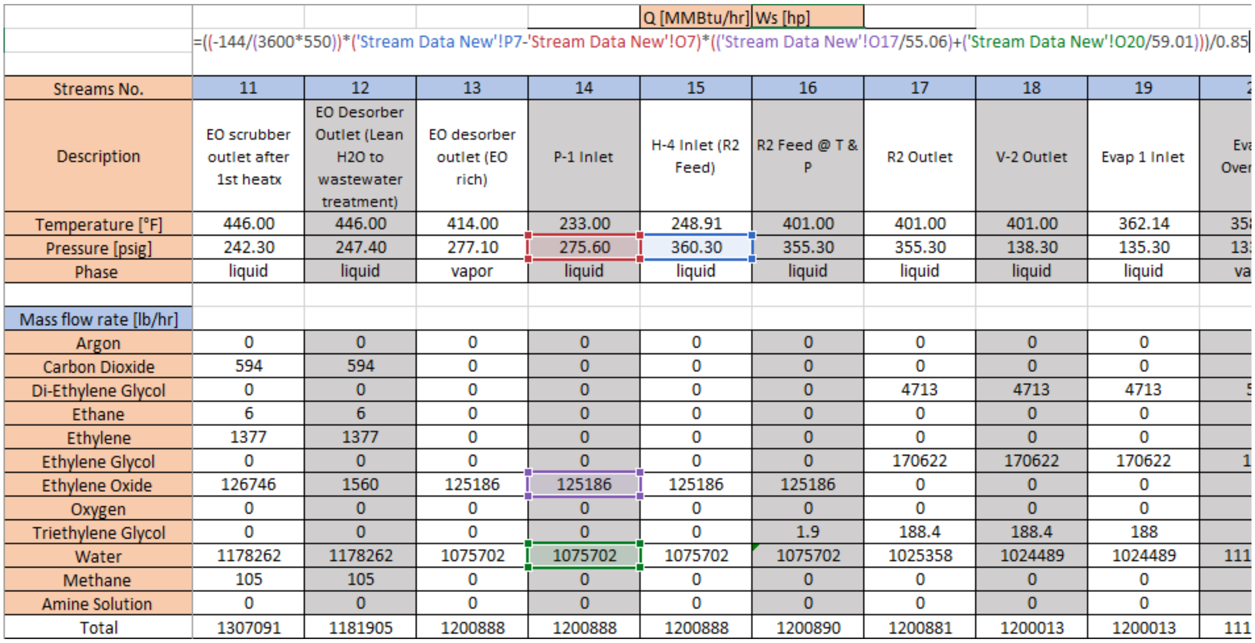
Comp-onent	Name		Liquid Phase Mole Fraction, x_i	Activity coefficient γ_i	P^s_i	Partial Pressure, p_i	Vapor Phase Mole Fraction, y_i	Vapor Phase Mole Fraction Calculated		K_i
					0	0				
1	Ethylene glycol		0.8172	1.000	60.63721	49.552	0.3303	0.0000	1.09E-01	0.40
2	Diethylene glycol		0.0131	1.000	17.40520	0.228	0.0015	0.0000	2.26E-06	0.12
3	Triethylene glycol		0.0004	1.000	5.83355	0.002	0.0000	0.0001	1.84E-09	0.04
4	Water		0.1694	1.000	591.72036	100.220	0.6681	0.9999	1.10E-01	3.94
					Total P:	150.0014	1.0000	Pressure error	1.92E-05	

7. Auxiliary Equipment Energy Balances

7.1. Pumps

7.1.1. $$Ws = -\frac{m\Delta P}{\eta * \rho}$$

- The expression comes from a reduced form of the energy balance for an adiabatic pump. All pumps are assumed to have an efficiency of 85%



				Q [MMBtu/hr]	Ws [hp]				

=((-144/(3600*550))*('Stream Data New'!P7-'Stream Data New'!O7)*(('Stream Data New'!O17/55.06)+('Stream Data New'!O20/59.01)))/0.85

Streams No.	11	12	13	14	15	16	17	18	19	2
Description	EO scrubber outlet after 1st heatx	EO Desorber Outlet (Lean H2O to wastewater treatment)	EO desorber outlet (EO rich)	P-1 Inlet	H-4 Inlet (R2 Feed)	R2 Feed @ T & P	R2 Outlet	V-2 Outlet	Evap 1 Inlet	Eva Over
Temperature [°F]	446.00	446.00	414.00	233.00	248.91	401.00	401.00	401.00	362.14	35
Pressure [psig]	242.30	247.40	277.10	275.60	360.30	355.30	355.30	138.30	135.30	13
Phase	liquid	liquid	vapor	liquid	liquid	liquid	liquid	liquid	liquid	va
Mass flow rate [lb/hr]										
Argon	0	0	0	0	0	0	0	0	0	
Carbon Dioxide	594	594	0	0	0	0	0	0	0	
Di-Ethylene Glycol	0	0	0	0	0	0	4713	4713	4713	5
Ethane	6	6	0	0	0	0	0	0	0	
Ethylene	1377	1377	0	0	0	0	0	0	0	
Ethylene Glycol	0	0	0	0	0	0	170622	170622	170622	1
Ethylene Oxide	126746	1560	125186	125186	125186	125186	0	0	0	
Oxygen	0	0	0	0	0	0	0	0	0	
Triethylene Glycol	0	0	0	0	0	1.9	188.4	188.4	188	
Water	1178262	1178262	1075702	1075702	1075702	1075702	1025358	1024489	1024489	111
Methane	105	105	0	0	0	0	0	0	0	
Amine Solution	0	0	0	0	0	0	0	0	0	
Total	1307091	1181905	1200888	1200888	1200888	1200890	1200881	1200013	1200013	111

- Above is a sample pump calculation, showing the calculation method used for P-1, P-2, & P-3.

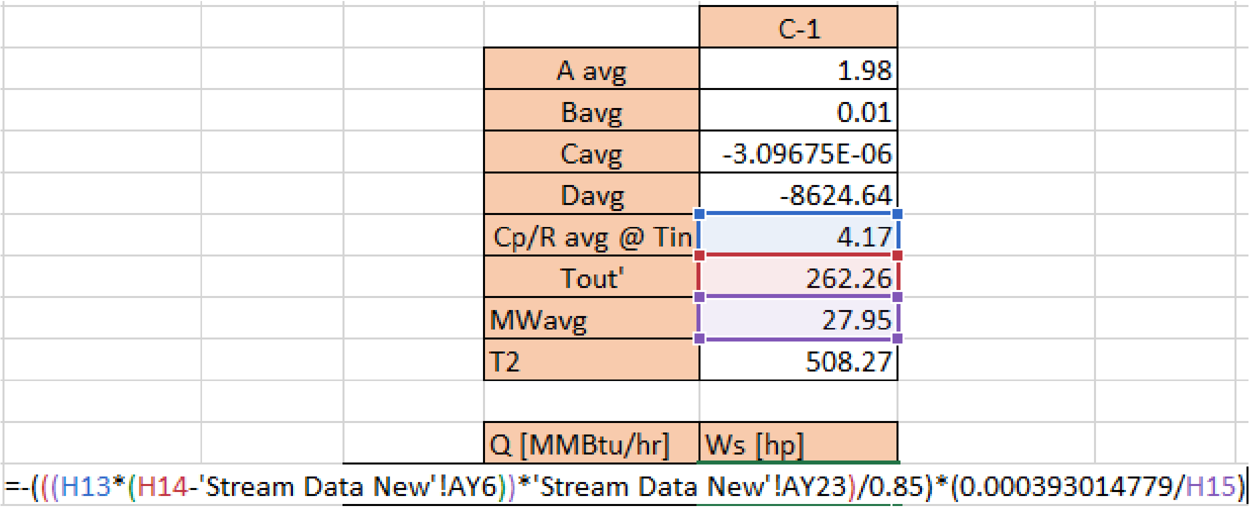
7.2. Compressors

7.2.1. $$T_2' = T_1\left(\frac{P_2}{P_1}\right)^{\frac{R}{C_p}}$$

7.2.2. $Ws(isentropic) = C_p(T_2' - T_1)$

7.2.3. $Ws = \frac{Ws(isentropic)}{\eta_{isentropic}}$

- For all compressors, an isentropic efficiency of 85% was assumed.



	C-1
A avg	1.98
Bavg	0.01
Cavg	-3.09675E-06
Davg	-8624.64
Cp/R avg @ Tin	4.17
Tout'	262.26
MWavg	27.95
T2	508.27
Q [MMBtu/hr]	Ws [hp]

```
=-(((H13*(H14-'Stream Data New'!AY6))*'Stream Data New'!AY23)/0.85)*(0.000393014779/H15)
```

- Above is a sample calculation showing the calculation method of C-1.

7.3. Heat Exchangers

7.3.1. Condensers

7.3.1.1. Total Condenser: $Q_c = D(R+1)\Delta H^{vap}$

7.3.1.2. Total Condenser: $Q_R = DR\Delta H^{vap}$

7.3.2. Reboilers

7.3.2.1. Partial Reboiler: $Q_R = BV_B\Delta H^{vap}$

7.3.3. Sensible Heat

7.3.3.1. $Q = \sum_i m_i \Delta H_i = \sum_i m_i \int_{Tin}^{Tout} Cp_i dT$

- The online database of Knovel was used for ΔH^{vap} for all the components. **[Knovel. "Engineering]**

Appendix III - Symbol & Nomenclature

Symbol	Nomenclature	Unit
A	Absorption Factor	-
ω	Acentric Factor	-
E_A	Activation Energy	Btu/lbmol
A_r	Arrhenius Pre-exponential	ft^3/lbmol-hr
V_B	Boil up Ratio	-
B	Column bottoms	lb/hr
D	Column distillate	lb/hr
z	Compressibility Factor	-
Z^0, Z^1	Compressibility Factor Lee Kesler Correlations	-
C_i	Concentration of component i	lbmol/ft^3
P_c	Critical Pressure	Bar
T_c	Critical Temperature	K
η	Efficiency	-
K	Equilibrium absorption/ stripping constant	-
x_B	Fraction of Light Key in the Bottoms	-
x_D	Fraction of Light Key in the Distillate	-
z_F	Fraction of Light Key in the Feed	-
R	Gas Constant	KJ/mol K

Cp	Heat Capacity	KJ/mol
C_{Pi}	heat capacity of component i	Btu/lbmol-°F
Q_c	Heat duty of a condenser	Btu/lb
Q_R	Heat duty of a reboiler	Btu/lb
$\dot{Q}$	Heat flow Negative = heat added Positive = heat removed	Btu/hr
ΔH_{Rx}	heat of reaction	Btu/lbmol
F_{io}	Initial flow rate of component i	lbmol/hr
v_o	Inlet total volume metric flow rate	ft^3/hr
L_c	Liquid Return	lb/hr
L_N	Molar flow of solute liquid on stage N	-
V_N	Molar flow of solute vapor on stage N	-
X_N	Moles of solute per mole of solute-free liquid on stage N	-
Y_N	Moles of solute per mole of solute-free vapor on stage N	-
P	Pressure	psig
k	Rate constant	ft^3/lbmol-hr
r_i	Rate reaction of component i	lbmol/ft^3-hr
P_r	Reduced Pressure	-
T_r	Reduced Temperature	-
T_R	Reference temperature	°F

R	Reflux rate	-
P^{sat}	Saturation Pressure	Bar
L’	Solute-free liquid	-
V’	Solute-free vapor	-
H_i^o	Standard enthalpy of component i	Btu/lbmol
S	Stripping Factor	-
T	Temperature	°F
W	Work	hp
U_o	Overall mass transfer coefficient	Btu/hr-ft^2-F
$LMTD$	Log Mean Temperature Different	-
L	Length of equipment	ft
r	Radius of equipment	ft
ΔH_{Rxi}	Change in heat of reaction	KJ/Kmol
C_{Pi}	Constant heat capacity	KJ/Kmol-K
M&S Index	Marshall & Swift Index	
F_C	Cost factor	
F_t	Tray type cost factor	
F_m	Material cost factor	
F_P	Pressure cost factor	
P_{HPS}	Price of HP Steam	$/Mlb
P_F	Price of boiler fuel	$/MMBtu
dH_b	Steam heating rate	MMBtu/lb
η_B	Boiler efficiency	

P_{BFW}	Price of boiler feed water	$/Mlb

Appendix IV - Problem Statement

This year's project is the design of an ethylene glycol plant via ethylene oxide based on ethylene feedstock with 99.9 wt% of Ethylene and 0.1 wt% of Ethane. The overall production is 700-kilo Tons per Annum (kTA) EG. This process also results in the formation of byproducts which mainly include di-ethylene glycol (DEG) and triethylene glycol (TEG). The project objective is to successfully achieve the total production quantity and product quality using appropriate unit operations.

Appendix V – MSDS

1. Oxygen: www.airgas.com/msds/001043.pdf
2. Ethane: www.airgas.com/msds/001024.pdf
3. Ethylene: www.airgas.com/msds/001022.pdf
4. Argon: www.airgas.com/msds/001004.pdf
5. Ethylene Oxide: www.airgas.com/msds/001081.pdf
6. Diethylene Glycol – Ethylene Glycol – Triethylene Glycol – Water: www.airgas.com/msds/026955.pdf
7. Methane: www.airgas.com/msds/001033.pdf
8. Carbon Dioxide: www.airgas.com/msds/001013.pdf
9. Ethanolamine: www.fishersci.com/store/msds?partNumber=M2511&productDescription=ETHANOLAMINE+PURIFIED+1L&vendorId=VN00033897&countryCode=US&language=en