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Hazard and Operability Analysis of an Ethylene Oxide Production Plant

Samantha Ciricillo
University of South Carolina, sammy.ciricillo@gmail.com

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By

Samantha Ciricillo

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Approved:

Dr. Thomas Stanford
Director of Thesis

Dr. Vincent Van Brunt
Second Reader

Steve Lynn, Dean
For South Carolina Honors College

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Thesis Summary

The purpose of this work was to evaluate potential hazards and failures as part of the design and economic analysis for a chemical plant that would produce 150,000 tons of ethylene oxide per year[1]. The Hazard and Operability (HAZOP) method of analysis was used to accomplish this goal. This method of hazard analysis involves brainstorming potential errors in a system by examining each element of each process unit in full detail. This project was focused on the reactor unit because the reactor has several important parameters that could fail, resulting in safety issues within the system. Input for this analysis was received from the other members of the process team: Justin Brown, Alyssa Matarazzo, and Kyle Tynan as well as faculty mentors Dr. Thomas Stanford and Dr. Vincent Van Brunt.

Through this analysis, many areas of concern for plant safety were found such as the ratio of hydrocarbon to oxygen causing an explosion hazard in the reactor, and the buildup of pressure in the reactor causing equipment failure. Additionally, safety precautions have been suggested such as adding a pressure relief system to the reactor, implementing controls on process parameters such as temperature and pressure, and writing emergency shutdown procedures in the case of system malfunction. These safety precautions are important for protecting the employees of the plant and the surrounding community.

Introduction

The goal of this report was to complete a detailed Hazard and Operability (HAZOP) analysis of the ethylene oxide production plant to complement the design and economic analysis of the plant conducted by the design group consisting of: Justin Brown, Samantha

Ciricillo, Alyssa Matarazzo, and Kyle Tynan[1]. The ethylene oxide plant was designed based on extensive research into industrial practices as well as literature on the chemistry and chemical kinetics of the direct oxidation of ethylene using a silver supported alumina oxide catalyst[2]. The chemical plant was designed to produce approximately 150,000 tons per year of ethylene oxide. The process was modeled using the Aspen HYSYS program and the process flow diagram was considered for this analysis.

Process Description

Ethylene oxide can be produced from ethylene in a number of ways; however, the most common industrial practice is to form ethylene oxide through the direct oxidation of ethylene with pure oxygen[2]. The reactant streams include a mixture of light hydrocarbons that is 94% ethylene as well as 99.5% pure oxygen[1]. The product stream will be mostly pure ethylene oxide as well as a waste liquid stream and vent gas streams. The by-products of this process are mostly water and carbon dioxide[2]. The process flow diagram for the process can be found in Appendix A and is taken directly from the Aspen HYSYS model simulation.

Table 1: Component List for Hydrocarbon Reactant Stream

Component	Mole Fraction
Methane	0.02
Ethylene	0.94
Ethane	0.03
Propylene	0.007
Propane	0.003

This process begins by separating the mixture of light hydrocarbons that includes methane, ethane, ethylene, propane and propene in order to get a high purity of ethylene[1]. The mole fractions of each component in the stream can be found in Table 1. This separation involves two distillation columns in series to remove the methane in the first column and the ethane, propylene and propane in the second from the material steam. After these separations, the stream is mixed with the pure oxygen and a recycle stream. Then, this reactant stream is fed into the reactor. In the reactor, three main reactions are occurring, which are the reactions considered in the model. The main reaction is the direct oxidation of ethylene to ethylene oxide. Additionally, ethylene and ethylene oxide undergo complete combustion to form carbon dioxide and water[1]. The reactor is a plug flow reactor with silver supported alumina oxide catalyst inside the tubes. This catalyst is proven to enhance the direct oxidation reaction.

After the reactor, the stream goes into an absorber. This separates most of the vent gases (carbon dioxide, oxygen and ethylene) from the water and ethylene oxide. The water and ethylene oxide mixture then goes through a refining process to remove the water and remaining vent gases, so the product is 99.73% pure ethylene oxide. The vent gases are treated in an amine absorber to remove carbon dioxide and then recycled to the reactor to react any remaining ethylene and oxygen[1]. During the process, it is important to pay attention to the lower and upper flammability limits of ethylene to avoid potential explosion hazards. At 25 °C and 1 atmosphere, the lower flammability limit for ethylene is 2.79% and the upper flammability limit for ethylene is 22.30%. The lower flammability limit for ethylene at the reactor temperature (240 °C) and pressure (2100 kPa) is 3.27%, while the upper flammability limit for ethylene at these conditions is 49.48%. The calculations for this data can be found in Appendix C.

Implementation of HAZOP Study

HAZOP analysis is a well-accepted and effective tool used extensively in industry. It is a formal procedure to identify hazards in a chemical production plant as well as determining precautions to prevent these hazards[3]. A HAZOP analysis is a structured and systematic evaluation of a planned process in order to assess potential risks in the process. The ultimate goal of this work was to determine potential hazards and safety issues in the design and implement actions to improve the safety of this process and protect the lives of those who work in the plant.

Description of HAZOP Methodology[3],[4]

The basic idea of the HAZOP methodology is to brainstorm in a controlled, methodical fashion in order to consider all potential operational failures that can occur in a chemical process[3]. The first step was to gather a team of people composed of a cross section of experienced professionals from different backgrounds[3]. A HAZOP analysis is always done in a group[4]. Because this work was conducted in an academic setting, the analysis was mainly done individually with some input from peers and mentors as detailed in the section labeled "Time of HAZOP Study and Participants of HAZOP Study Group". This procedure typically starts by looking at an up-to-date process flow diagram, such as the one in Appendix A. Other process information such as material and energy balances, materials of construction, and equipment specifications were also considered.

Next, the process was considered as a whole to determine which process unit has the highest potential for hazards. It was determined that the plug flow reactor would be the best unit to look at since it is a key unit in the process and has many process parameters. Once the study node was chosen to be the reactor, the intent of the study node was identified[3]. The intent of the reactor is to facilitate the reaction of ethylene and oxygen to produce ethylene oxide using a silver supported alumina catalyst for efficiency.

Once the initial steps were finished, process parameters for the reactor were determined. These parameters included ethylene flow, oxygen flow, ethylene oxide flow, temperature, pressure, reactor volume, etcetera, which were determined during the design of the plant. These parameters were used to describe potential failures in the process that could cause safety issues. Then, guide words were applied to each process parameter to describe specific failures that may occur. These guide words are described in Table 2. Not every guide word was applicable to every process parameters, and some combinations did not produce potential hazards. This procedure could produce hundreds of combinations, but only those that were brainstormed and could produce potential hazards were considered. The combinations of guide words and process parameters are described more fully in the "Deviation" column of the HAZOP analysis table, which can be found in Appendix B.

Table 2: Guide Words for HAZOP Analysis[3]

Guide words	Meaning	Comments
NO, NOT, NONE	The complete negation of the intention	No part of the design intention is achieved, but nothing else happens.
MORE, HIGHER, GREATER	Quantitative increase	Applies to quantities such as flow rate and temperature and to activities such as heating and reaction.
LESS, LOWER	Quantitative decrease	Applies to quantities such as flow rate and temperature and to activities such as heating and reaction.
AS WELL AS	Qualitative increase	All the design and operating intentions are achieved along with some additional activity, such as contamination of process streams.
PART OF	Qualitative decrease	Only some of the design intentions are achieved, some are not.
REVERSE	The logical opposite of	Most applicable to activities such as flow or chemical reaction. Also applicable to substances, for example, poison instead of antidote.
OTHER THAN	Complete substitution	No part of the original intention is achieved—the original intention is replaced by something else.
SOONER THAN	Too early or in the wrong order	Applies to process steps or actions.
LATER THAN	Too late or in the wrong order	Applies to process steps or actions.
WHERE ELSE	In additional locations	Applies to process locations, or locations in operating procedures.

Once the combinations of guide words and parameters were chosen, possible causes were considered. Many different occurrences could be the cause of the same failure, so a list of potential causes was created in the analysis table. Additionally, a list of possible consequences for each guide word/parameter combination was also added to the analysis table. These two columns of the table were considered to form the final column of the analysis table, “Actions Required”. The final HAZOP analysis table can be found in Appendix B of this report. If this ethylene oxide plant were to be actually conducted based on the proposed design, the required actions would need to be finished in a timely manner, and all process hazard analyses would need to be updated every 3 years[4].

Time of HAZOP Study and Participants of HAZOP Study Group

This HAZOP analysis took place during the period of January to April of 2019. The analysis was completed concurrently with the design of the process and was continually updated as the process design was updated. This analysis was mainly led and completed by Samantha Ciricillo, but includes input from design team members Justin Brown, Alyssa Matarazzo, Kyle Tynan, and faculty mentors Dr. Thomas Stanford and Dr. Vincent Van Brunt. Mostly informal meetings were held throughout the period of HAZOP analysis to gain input from the group members and mentors.

Major Results and Findings

The HAZOP analysis identified as the main concern for the plant to be the ratios of ethylene and ethylene oxide to oxygen in the reactor. If the lower flammability limit or upper flammability limit of ethylene was reached in the reactor, then any spark near the system could cause an explosion in the plant. The concentrations of oxygen, ethylene, and ethylene oxide as well as their ratios should be monitored by the control system in the plant.

Assurance of proper flows within the piping is also an important factor, and flow meters should be placed throughout the plant to monitor the streams. Emergency procedures should be put into place for shutdown in the event of any issues with these ratios or with feed or product stream malfunctions. These procedures will be crucial in protecting the lives of the plant personnel.

Additionally, over-pressurization is a concern in the reactor. Many factors can cause pressure to build up in the reactor unit, such as a runaway reaction or lack of product flow out of the reactor. For this reason, a pressure relief system in the reactor is crucial. The implementation of this system is described in the "Future Work" section of the report. A pressure relief system should be implemented in the separation unit as well to protect from a potential explosion. A situation like this occurred in 1991 at the Union Carbide ethylene oxide plant in Sea Drift, TX where the separation unit over-pressured and caused extensive damage[5]. The pressure of the system should be monitored using a controls system, and pressure relief measures should be put into place. Additionally, there should be an emergency shutdown procedure put into place in case of a buildup of pressure.

The temperature of the system should also be monitored through a control system and controlled through heating or cooling jackets on the vessels, especially the reactor. Temperature is important for the kinetics of the reaction and for proper heat of reaction to be met. Additionally, temperature is important for pressure regulation in the reactor. Lack of temperature control could lead to an uncontrolled reaction, which is especially unsafe when dealing with oxygen and hydrocarbons that could lead to explosions in uncontrolled ratios. Emergency shutdown procedures are important in the event of temperature increase above a maximum or decrease below a minimum, as well as a loss of temperature control.

Finally, it is important to do routine checks and maintenance of the piping, reactor, flow meters, valves, control system, and any involved units to assure proper function. Buildup of material in the reactor or piping could cause issues with the reaction or corrosion. Additionally, leaks are possible if the equipment is not checked routinely for damage or corrosion. Procedures should be put in place for the occurrence of leaks or the necessity of non-routine maintenance to assure the safety of the operators, engineers, and other staff in the plant. Preventative maintenance should be performed on equipment every 6 months to prevent failure of the system or the equipment materials. An updated HAZOP analysis is necessary for the equipment anytime an update is made or there is a malfunction after which the equipment must be adjusted and restarted. This should be at least at a frequency of every 3 years.

Future Work

The design of this plant is completely theoretical; therefore, a plant will not be built or run in the future based on this design. For this reason, the "Actions Required" detailed in the HAZOP analysis chart (Appendix B) were not implemented in the design. However, it is still important to consider how these actions would be implemented. Some of the actions would be added to the design far before the plant is running. For example, relief sizing is an important aspect for safety. Every unit would need to be considered for a different type of relief system, and then that relief system would need to be sized for that unit[6]. For example, the reactor would likely need a spring-loaded relief valve because the mixture of chemicals is not corrosive by nature and is not acutely toxic[3]. The pressure drop between the vessel and the valve should be no more than 3% of the set pressure, so no more than 63 kPa[3],[6]. The relief valve could be added to the HYSYS simulation and sized in HYSYS[7]. The mixture should go to a properly-sized flare drum or series of flare drums to be combusted in a controlled environment to form CO_2 and water, which are not hazardous[3]. These relief system considerations would need to be continued for every unit in the process.

Other pre-planned precautions include many of the controls of the plant. A control system should be established in the plant in order to monitor temperature, pressure, flow, concentration, and other process parameters that would affect the safety of the plant. This system allows for safety procedures to be implemented as well as for the process to be monitored, which is helpful for business in the long run. If there are reoccurring issues in a process, the engineers can take this control data, investigate the underlying issue, and suggest new solutions. Control systems can be linked to alarms and warnings in case plant personnel need to evacuate in the event of a leak or overpressure.

In addition to these pre-planned safety features in the plant, it is of utmost importance that plans be put into place for proper safety operating procedures to be followed. These plans need to include standard operating procedures, routine equipment checks, routine equipment maintenance plans, and emergency shutdown procedures. Having these procedures and teaching them to all plant personnel reduces the chance of a catastrophic incidence occurring in the plant. If everybody is aware of possible failures in the plant and how to mitigate the effects of those issues, then the plant environment is safer. New hires should go through extensive safety training, and each employee should receive continued safety training throughout his or her entire time at the plant. If everyone is committed to doing their part for the safety of the plant, emergencies can be minimized for everyone.

Conclusions

Through this process, it has become clear that safety is a crucial consideration in the design of a chemical plant. A thorough safety review and hazard analysis should be performed before any plant is built as well as after the plant is complete and ready for startup. So many disasters are possible, and awareness is the first step to preventing these disasters from occurring. If all plant personnel are on board with making the plant safer, then the probability of a catastrophe can be reduced. However, it is important that throughout the design process, design engineers should consider how the plant can fail and include design features to minimize those failures. The HAZOP methodology is a great tool to bring awareness to these potential failures and consider how to prevent them. However, the methodology is only as thorough as the committee performing the analysis, so it is important that those personnel are responsible and diligent in their analysis. Overall, this HAZOP analysis brings to focus the importance of safety analysis as a part of the conceptual design of any chemical process.

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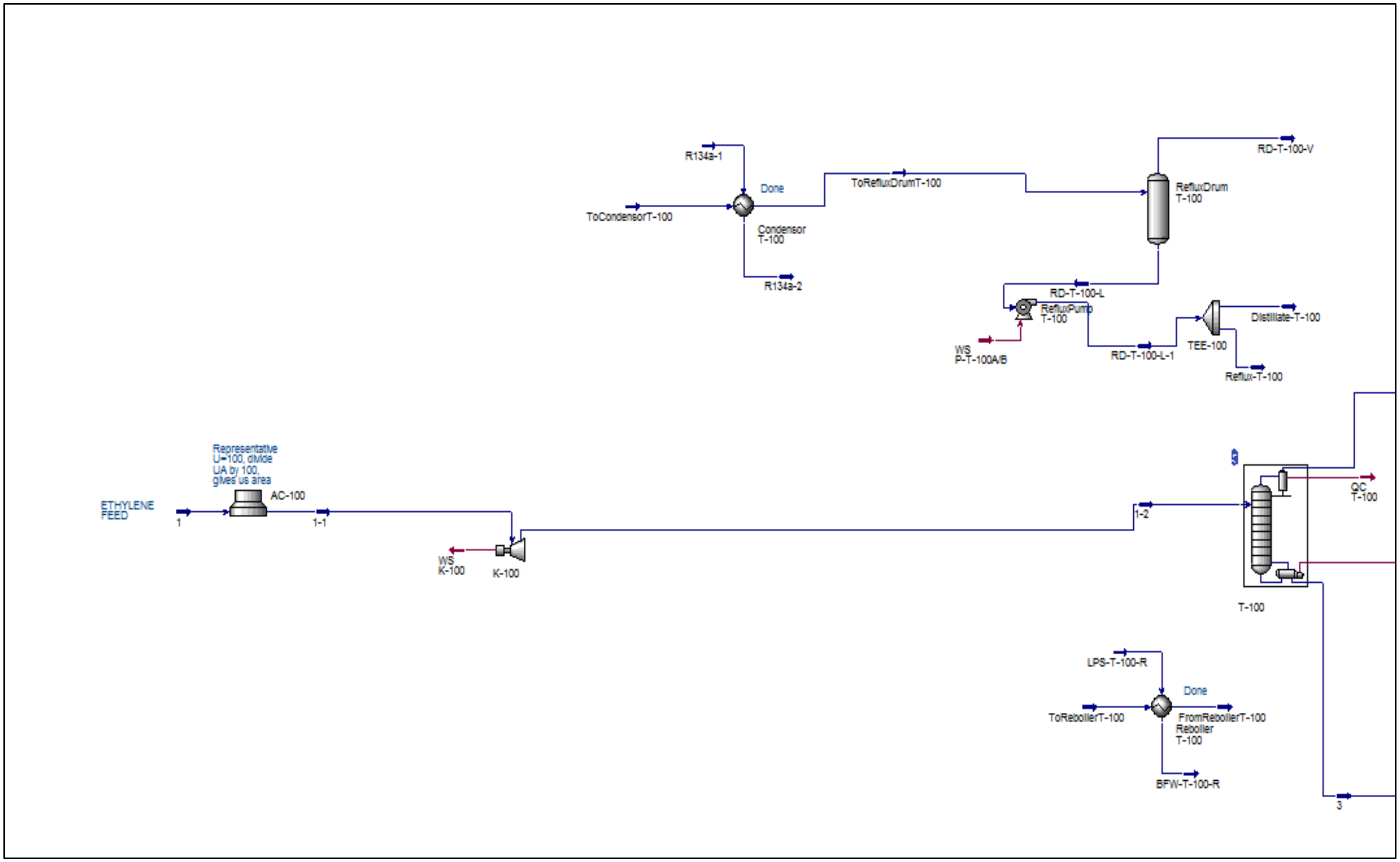
Appendix A: Process Flow Diagrams and Equipment List

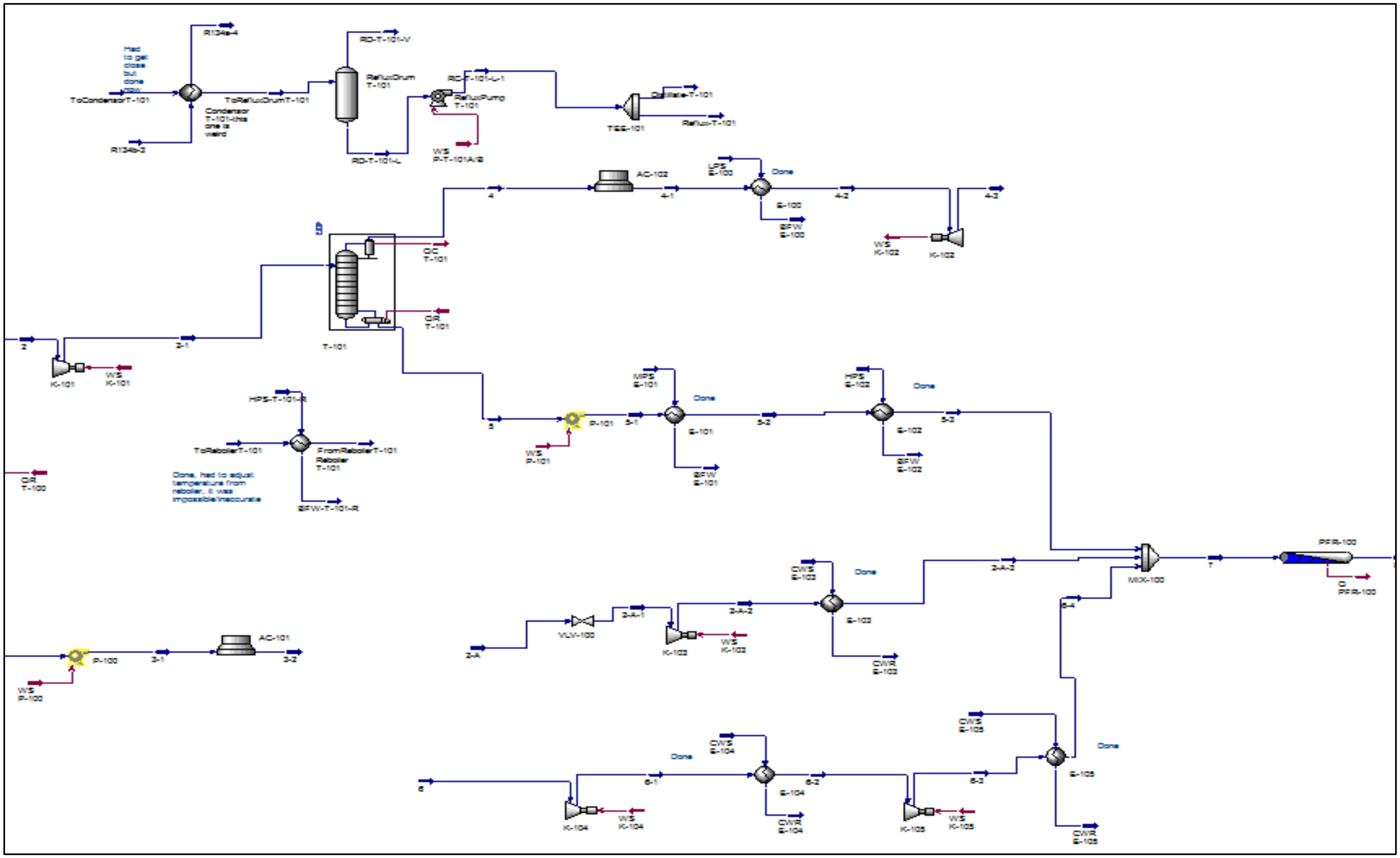
Equipment List:

Equipment:	Equipment:	Equipment:
Air Heaters	Compressors/Expanders	Reflux Drums
AC-100	K-100	RD T-100
AC-101	K-101	RD T-101
AC-102	K-102	RD T-103
Condensors	K-103	Reflux Pumps
C T-100	K-104	RP T-100
C T-101	K-105	RP T-101
C T-103	K-106	RP T-103
Heat Exchangers	Mixers	Towers
E-100	MIX-100	T-100
E-101	MIX-100-A	T-101
E-102	MIX-101-A	T-102
E-103	Pumps	T-103
E-104	P-100	T-100-A
E-105	P-101	T-101-A
E-106	P-102	Vessel
E-106-2	P-100-A	V-100-A
E-107	Reactor	Valves
E-108	PFR-100	VLV-100
E-100-A	Reboilers	VLV-101
E-101-A	R T-100	VLV-102
E-102-A	R T-101	VLV-100-A
E-103-A	R T-103	
E-104-A	R T-101-A	

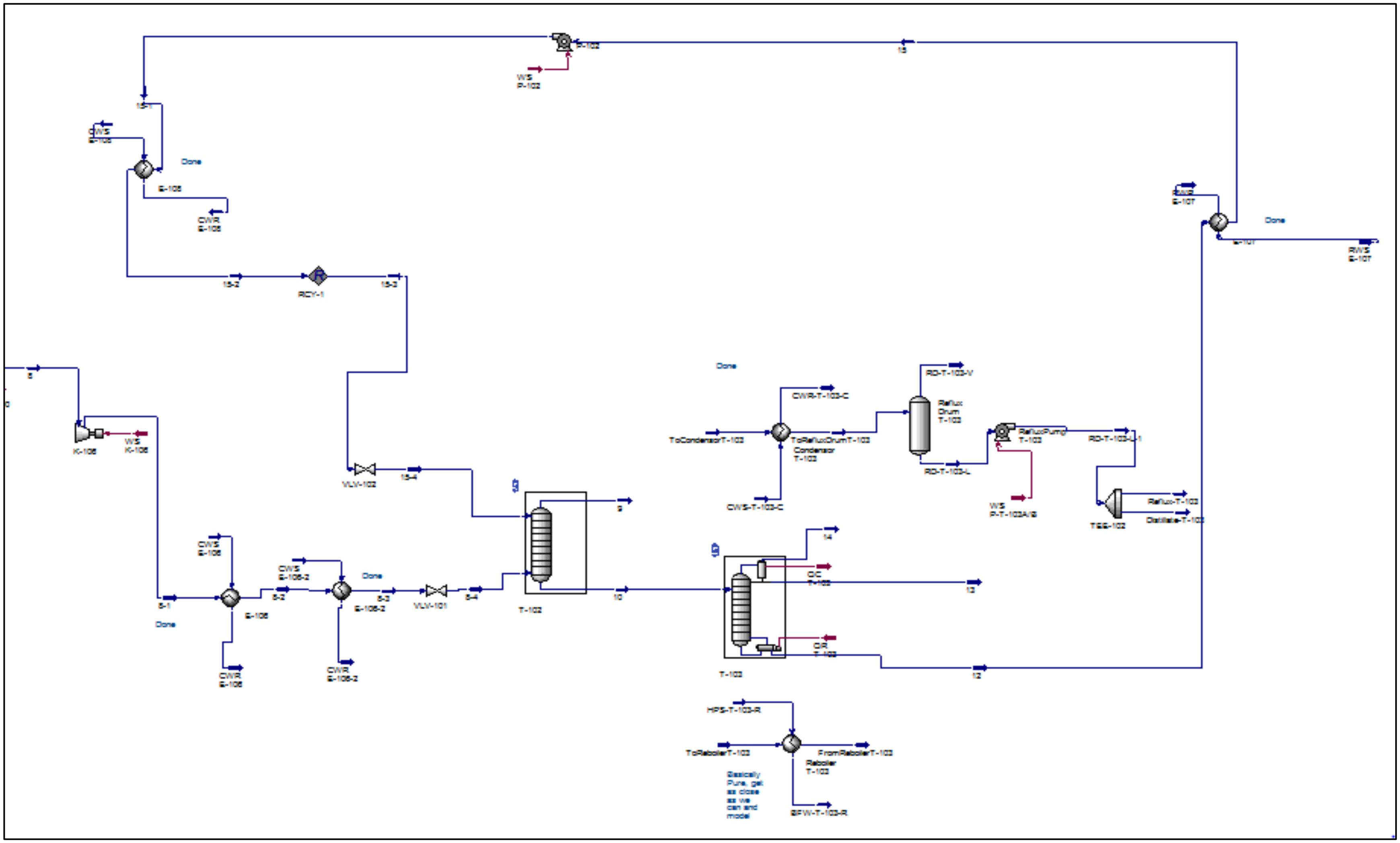
Ethylene Oxide Process Flowsheet Part 1:



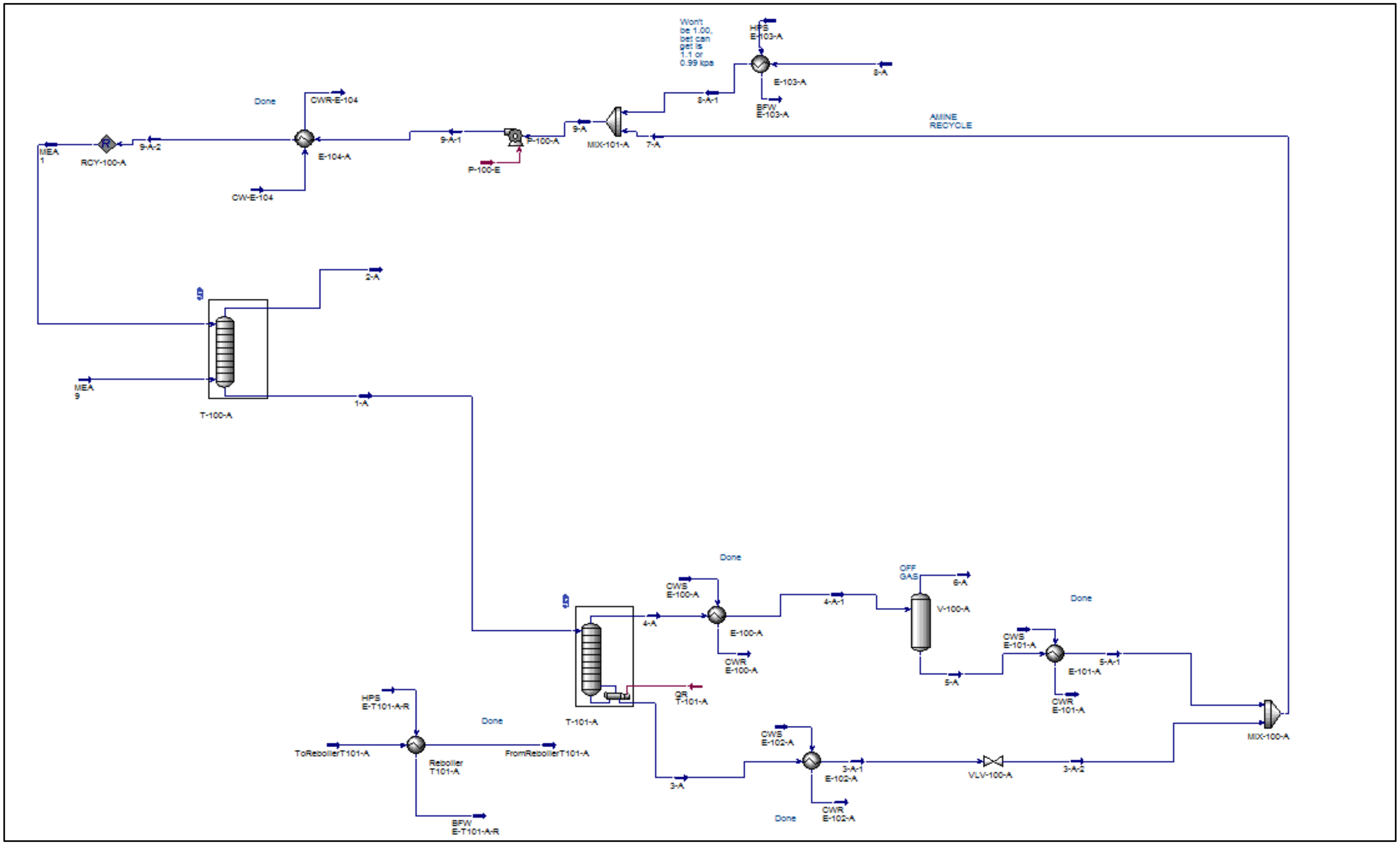
Ethylene Oxide Process Flowsheet Part 2:



Ethylene Oxide Process Flowsheet Part 3:



Amine Absorber Flowsheet:



Appendix B: Ethylene Oxide Production Plant HAZOP Analysis Worksheet

Item	Study Node	Guide Word	Process Parameter	Deviations	Possible Consequences	Potential Causes	Actions Required
1.1	Reactor	None	Ethylene Flow	No ethylene flow	1. Excess oxygen could react with any possible fuel sources in the reactor causing uncontrolled combustion	1. Clog in ethylene line 2. Valve failed closed in ethylene line 3. Not enough ethylene in storage	1. Routinely check ethylene lines for build up or corrosion 2. Routinely check the level of ethylene storage tank 3. Implement safe shutdown of the reactor when feed streams fail
1.2	Reactor	Higher	Ethylene Flow	Too much ethylene flow	1. Could reach the UFL and cause an explosion 2. Pressure could build up in tank causing an explosion 3. Ethylene could leak into plant	1. Flow rate input too high 2. Valve failed opened in ethylene line	1. Add interlocks in controls to limit flow rate below a maximum 2. Set valves to fail closed 3. Monitor ratio of oxygen to ethylene to keep from reaching UFL 4. Add a PRV into tank 5. Routinely check ethylene lines for leaks/have leak procedure in place 6. Implement safe shutdown of the reactor when feed

							streams malfunction
1.3	Reactor	Lower	Ethylene Flow	Too little ethylene flow	1. Could reach the LFL and cause an explosion	1. Clog in ethylene line 2. Not enough ethylene in storage	1. Routinely check ethylene lines for build up or corrosion 2. Routinely check the level of ethylene storage tank 3. Monitor ratio of oxygen to ethylene to keep from reaching LFL 4. Implement safe shutdown of the reactor when feed streams fail
1.4	Reactor	Reverse	Ethylene Flow	Ethylene flow reverses	1. Pressure could build up in pipes and storage tank causing an explosion	1. High pressure in reactor could cause flow to reverse	1. Add a PRV to the tank 2. Add check valves to ethylene line to prevent back flow 3. Implement safe shutdown of the reactor when feed streams malfunction
2.1	Reactor	None	Oxygen Flow	No oxygen flow	1. Ethylene is extremely flammable and could combust if it comes in contact with a spark	1. Clog in oxygen line 2. Valve failed closed in oxygen line 3. Not enough oxygen in storage	1. Routinely check ethylene lines for build up or corrosion 2. Routinely check the level of ethylene storage tank

							3. Implement safe shutdown of the reactor when feed streams fail
2.2	Reactor	Higher	Oxygen Flow	Too much oxygen flow	1. Could reach LFL and cause explosion 2. Pressure could build up in tank and cause explosion 3. Oxygen could leak into plant	1. Flow rate input too high 2. Valve failed opened in oxygen line	1. Add interlocks in controls to limit flow rate below a maximum 2. Set valves to fail closed 3. Monitor ratio of oxygen to ethylene to keep from reaching LFL 4. Add a PRV into tank 5. Routinely check oxygen lines for leaks/have leak procedure in place 6. Implement safe shutdown of the reactor when feed streams malfunction
2.3	Reactor	Lower	Oxygen Flow	Too little oxygen flow	1. Could reach UFL and cause explosion	1. Clog in oxygen line 2. Not enough oxygen in storage	1. Routinely check oxygen lines for build up or corrosion 2. Routinely check the level of oxygen storage tank 3. Monitor ratio of oxygen to ethylene to keep from reaching LFL

							4. Implement safe shutdown of the reactor when feed streams fail
2.4	Reactor	Reverse	Oxygen Flow	Oxygen flow reverses	1. Pressure could build up in pipes and storage tank causing an explosion or leak	1. High pressure in reactor could cause flow to reverse	1. Add a PRV to the tank 2. Add check valves to ethylene line to prevent back flow 3. Implement safe shutdown of the reactor when feed streams malfunction
3.1	Reactor	None	Product Flow	No product flow	1. Pressure could build up in the reactor and could cause explosion 2. Ethylene or ethylene oxide could combust with oxygen in the reactor	1. Clog in product line 2. Valve failed closed in product line	1. Regularly check product line for build up or corrosion 2. Make sure product line valves are fail open 3. Add PRV to the reactor 4. Implement safe shutdown of the reactor when product stream fails
3.2	Reactor	Higher	Product Flow	Too much product flow	1. Ethylene oxide could leak into plant 2. Separator pressure may increase 3. Unreacted reactants could flow out of the reactor too quickly and would be in an uncontrolled ratio	1. More reacted than anticipated 2. Product flow rate set too high 3. Valve failed open in product line 4. Pressure in reactor too high	1. Set controls for product flow rate to limit it to a maximum 2. Routinely check for leaks in the product line 3. Add a PRV to separator 4. Add PRV to reactor

					that could cause an explosion		5. Implement safe shutdown of the reactor when product stream malfunctions
3.3	Reactor	Lower	Product Flow	Too little product flow	1. Pressure in reactor could build up and cause explosion	1. Clog in product line 2. Valve closed partially open	1. Regularly check product line for build up or corrosion 2. Make sure product line valves are fail open 3. Add PRV to reactor Implement safe shutdown of the reactor when product stream fails
3.4	Reactor	Reverse	Product Flow	Product flow reverses	1. Pressure could build up in the reactor and could cause explosion 2. EO could backflow into ethylene or oxygen lines	1. Pressure in reactor could be too low causing reverse product flow	1. Monitor reactor pressure on DCS system and have emergency procedures in place 2. Add PRV on reactor 3. Add check valves to product lines, ethylene lines and oxygen lines 4. Implement safe shutdown of the reactor when product stream malfunctions
4.1	Reactor	Higher	Pressure	Pressure too high	1. Reactor material could weaken	1. Uncontrolled reaction occurs	1. Monitor reactor pressure on DCS system and have

					causing leak or explosion	2. Too much of a certain flow coming into reactor 3. Too little product flow out of reactor 4. Temperature increases dramatically	emergency shutdown procedures in place 2. Add valve controls onto product and reactant lines 3. Monitor reactor temperature on DCS and have emergency shutdown procedures in place 4. Add PRV to reactor 5. Add thermal control jacket to reactor
4.2	Reactor	Lower	Pressure	Pressure too low	1. EO line could back flow into the reactor 2. Uncontrolled amounts of oxygen or ethylene could go into the reactor and react without supervision	1. Not enough reactant coming into the reactor 2. Too much product flow leaving the reactor 3. Temperature dramatically decreases 4. Reaction is less than anticipated	5. Monitor reactor pressure on DCS system and have emergency shutdown procedures in place 6. Add valve controls onto product and reactant lines 7. Monitor reactor temperature on DCS system and have emergency shutdown procedures in place 8. Add thermal control jacket to reactor
5.1	Reactor	Higher	Temperature	Temperature too high	1. Reactor could overheat	1. Incoming reactant temperature is too high	1. Add thermal control jacket to reactor

					2. Materials could decompose into unknown or unwanted chemicals 3. Reactor pressure could increase	2. Reaction thermodynamics proceed in an uncontrolled fashion	2. Monitor reactor temperature on DCS system and have emergency shutdown procedures in place 3. Monitor reactor pressure on DCS system and have emergency shutdown procedures in place
5.2	Reactor	Lower	Temperature	Temperature too low	1. Reaction kinetics would be affected and the reaction would be unpredictable 2. Reactor pressure could decrease	1. Incoming reactant temperature is too low	1. Add thermal control jacket to reactor 2. Monitor reactor temperature on DCS system and have emergency shutdown procedures in place 3. Monitor reactor pressure on DCS system and have emergency shutdown procedures in place
6.1	Reactor	Less Than	Volume	Not enough volume in reactor	1. Reaction kinetics would be affected and the reaction would be unpredictable 2. Reactor pressure could increase	1. Build up of material inside the reactor would cause the available volume to decrease	1. Routinely check for buildup in the reactor and clean the reactor. 2. Monitor reactor pressure on DCS system and have emergency shutdown procedures in place

7.1	Reactor	None	Reaction	No reaction occurs	1. Ethylene and oxygen could combust causing pressure and temperature build up	1. Catalyst fouling or deactivation 2. Ignition temperature for reaction is not met at the reactor conditions	1. Routinely monitor catalyst for effectiveness 2. Monitor reactor pressure on DCS system and have emergency shutdown procedures in place 3. Monitor reactor temperature on DCS system and have emergency shutdown procedures in place
7.2	Reactor	Higher	Reaction	Higher conversion than expected	1. Too much EO would be formed causing pressure buildup in reactor 2. EO could also leak into the plant	1. Temperature is too high 2. Kinetics proceed uncontrolled	1. Control temperature through DCS and thermal jacket 2. Monitor the concentration of ethylene oxide in the product stream and have emergency shutdown procedures in place
7.3	Reactor	Lower	Reaction	Lower conversion than expected	1. Ethylene and oxygen would be in an uncontrolled ratio in the reactor	1. Temperature is too low 2. Kinetics proceed uncontrolled	1. Control temperature through DCS and thermal jacket 2. Monitor the concentration of ethylene oxide in the product stream and have emergency

							shutdown procedures in place
7.4	Reactor	Faster	Reaction	Reaction occurs too fast	1. EO could react with incoming oxygen and cause combustion	1. Temperature is too high 2. Kinetics proceed uncontrolled	1. Control temperature through DCS and thermal jacket 2. Monitor the concentration of ethylene oxide in the product stream and have emergency shutdown procedures in place
7.5	Reactor	Slower	Reaction	Reaction occurs too slow	1. Ethylene and oxygen would be in an uncontrolled ratio in the reactor	1. Temperature is too low 2. Kinetics proceed uncontrolled	1. Control temperature through DCS and thermal jacket 2. Monitor the concentration of ethylene oxide in the product stream and have emergency shutdown procedures in place
7.6	Reactor	As Well As	Reaction	Side reactions occur along with the anticipated reactions	1. Uncontrolled/unanticipated side reactions could cause unwanted products	1. Impurities in the reactants could cause side reactions	1. Purify the reactants as much as possible through separations 2. Monitor the concentration of ethylene oxide in the product stream and have emergency shutdown procedures in place

7.7	Reactor	Other Than	Reaction	Reactions other than those anticipated occur	1. Uncontrolled/unanticipated reactions could cause unwanted products	1. Impurities in the reactants could react 2. Ethylene could completely combust	1. Purify the reactants as much as possible through separations 2. Monitor the concentration of ethylene oxide in the product stream and have emergency shutdown procedures in place
8.1	Reactor	Higher	Ethylene Concentration	Concentration of ethylene is too high	1. This could reach an unsafe ratio of fuel to oxygen.	1. Issues in the oxygen feed system, a compressor fails for example	1. Implement safe shutdown of the reactor when feed streams fail 2. Routine checking of feed stream operability
8.2	Reactor	Lower	Ethylene Concentration	Concentration of ethylene is too low	1. This could reach an unsafe ratio of fuel to oxygen.	1. Impurities in stream could cause the concentration to be too low	1. Purify the reactants as much as possible through separations 2. Implement safe shutdown of the reactor when feed streams fail
9.1	Reactor	Higher	Oxygen Concentration	Concentration of oxygen is too high	1. This could reach an unsafe ratio of fuel to oxygen.	1. Issues in the ethylene feed system, a compressor fails for example	1. Implement safe shutdown of the reactor when feed streams fail 2. Routine checking of feed stream operability
9.1	Reactor	Lower	Oxygen Concentration	Concentration of oxygen is too low	1. This could reach an unsafe ratio of fuel to oxygen.	1. Impurities in stream could cause the concentration to be too low	1. Purify the reactants as much as possible through separations 2. Implement safe shutdown of the

								reactor when feed streams fail

Appendix C: Detailed Calculations

Lower and Upper Flammability Limits of Ethylene at Reactor Temperature and Pressure:

Ethylene is an unsaturated alkene, therefore the parameters to calculate the UFL and LFL are as follows[8]:

$$a = 0.4265$$

$$b = 3.41$$

Then the C_{st} value needs to be calculated[3]:

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$$

$$C_{st} = \frac{100}{1 + (\frac{mol\ O_2\ for\ combustion}{0.21})} = \frac{100}{1 + (\frac{3}{0.21})} = 6.54$$

Therefore, at T = 25°C and P = 2100 kPa[8]:

$$LFL = a \times C_{st} = 0.4265 \times 6.54 = 2.79\%$$

$$UFL = b \times C_{st} = 3.41 \times 6.54 = 22.30\%$$

To find these values at the reactor temp of 240°C, the heat of combustion is needed[9]:

$$\Delta H_c = -1411.20\ \frac{kJ}{mol} = -337.29\frac{kcal}{mol}$$

Therefore, at T = 240°C[3]:

$$LFL = LFL_{25} - \frac{0.75}{\Delta H_c}(T - 25) = 2.79 - \frac{0.75}{-337.29}(240 - 25) = 3.27\%$$

$$UFL = UFL_{25} + \frac{0.75}{\Delta H_c}(T - 25) = 22.30 + \frac{0.75}{-337.29}(240 - 25) = 21.82\%$$

The LFL does not change much with high pressure, but to find the UFL at the reactor pressure of P = 2100 kPa gauge = 2.201 MPa abs[3]:

$$UFL = UFL_{1\ atm} + 20.6(\log(P) + 1) = 21.82 + 20.6(\log(2.201) + 1) = 49.48\%$$

Therefore, at reactor temperature and pressure:

$$LFL = 3.27\%$$

$$UFL = 49.48\%$$