CHE654 – Plant Design Project #4
Semester 1, 2022

DESIGN OF AN ETHYLENE OXIDE PRODUCTION PROCESS

(Courtesy of the Department of Chemical Engineering at West Virginia University)

Introduction

Ethylene oxide (EO) is a major commodity chemical that is manufactured throughout the world. Ethylene oxide is a chemical used to make ethylene glycol (the primary ingredient in antifreeze). It is also used to make poly(ethylene oxide), and both the low molecular weight and high molecular weight polymers have many applications including as detergent additives. Because ethylene oxide is so reactive, it has many other uses as a reactant.

Your company believes that the market for ethylene oxide will increase significantly over the next few years. Therefore, they are looking at expansion of their ethylene oxide capacity. Your assignment is to design a new, grass-roots facility to produce 100,000 tonne/year of ethylene oxide in an 8000-hour year.

Ethylene oxide is produced by the catalytic oxidation of ethylene over a silver-containing catalyst. A side reaction oxidizes ethylene to carbon dioxide and water.

$$C_2H_4 + 0.5O_2 \rightarrow C_2H_4O \qquad \zeta_1$$

$$C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \qquad \zeta_2$$

where ζ_i is the extent of reaction of reaction *i*. The selectivity of these reactions is determined by processing conditions. In the normal operating range for the catalyst (225 to 275°C), lower single-pass conversion favors ethylene oxide production. A simplified process flow diagram for an EO process is shown in Figure 1. Your job is to analyze the simplified ethylene oxide production process, to suggest profitable operating conditions, and to write a final report summarizing your findings. Note that although you are to look for a "best" solution in your design, optimization is <u>NOT</u> required in this design project.

Process Description

Figure 1 is a preliminary process flow diagram (PFD) for the ethylene oxide production process. The raw material is ethylene, which may be assumed to be pure. Air is compressed in C-701 and mixed with the feed. The mixed feed is heated, vaporized, and superheated in a heat exchanger (E-701); and is then sent to the reactor (R-701) in which ethylene oxide (EO) is formed. The reactions that occur are shown later. The reactor effluent is cooled and partially condensed in a heat exchanger (E-702), and it is then sent to the separation section. In T-701, water is used to absorb the EO from the reactor effluent stream. The water and EO are then sent to a distillation column, T-702, where "pure" EO is produced in the top stream (distillate), with water in the bottom stream (bottoms). In T-701, the vapor stream leaving the top contains ethylene for recycle. However, nitrogen must be purged. The desired EO production rate is 100,000 tonne/year.

Process Details

Feed Streams

Stream 1: ethylene, from pipeline at 35 bar and 25°C, may be assumed pure

Stream 2: dried air, assumed to be 79 mol % nitrogen, 21 mol % oxygen, 1 atm, 25°C
excess air needed so that ethylene is ≤ 3 vol % (to be below flammability limit for safety purposes)

or use "pure" oxygen (99 wt % with 1 wt % nitrogen), 1 atm, 25°C
no concentration restriction because all concentrations within flammability limit (hence, there are safety issues, though it is done in industry)
oxygen to ethylene ratio is the same as when using air

Stream 9: pure water at 25°C, available at needed pressure

Effluent Streams

Stream 12: purge stream – may be burned as fuel gas – credit may be taken for LHV at $2.50/GJ

Stream 14: EO product, required 100,000 tonne/year. The required purity specification is 99.5 wt% ethylene oxide.

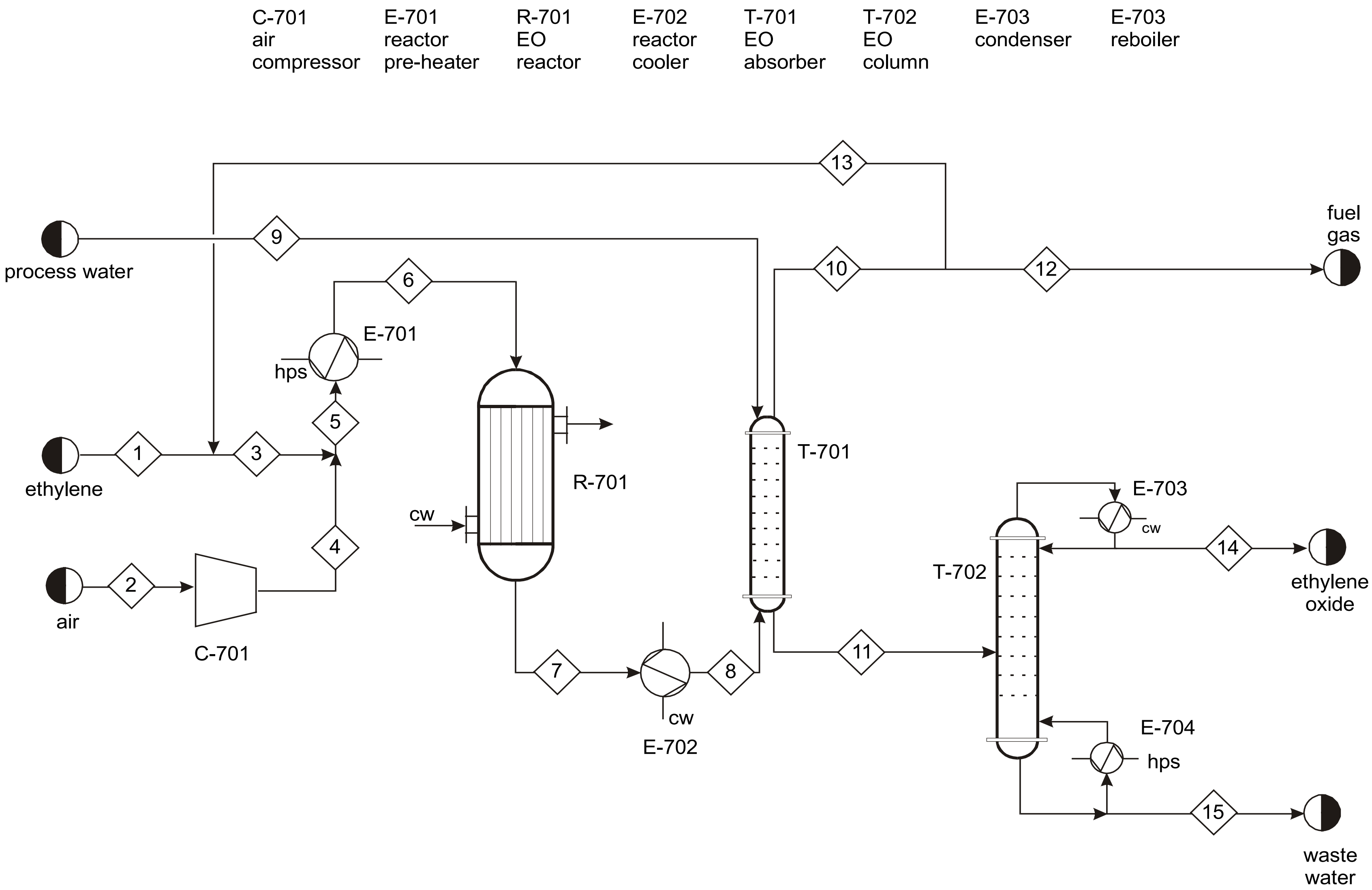

Figure 1: Process Flow Diagram for Ethylene Oxide Production

Stream 15: waste water stream, may be assumed pure in material balance calculations, is not pure, so there is a cost for its treatment

Equipment

Compressor (C-701)

The compressor increases the pressure of the feed air to the reactor pressure. The work for a compressor may be calculated as

$$W_s = 4.5RT_{in}\left[\left(\frac{P_{out}}{P_{in}}\right)^{0.286} - 1\right] \tag{1}$$

where the work is in kJ/kmol and the temperature is in Kelvin.

Heat Exchanger (E-701):

This unit heats, vaporizes, and superheats the feed to 240°C at the reactor pressure. The source of energy for heating must be above 240°C.

Reactor (R-701):

The following reactions are known to occur:

$$\underset{\text{ethylene}}{C_2H_4} + 0.5O_2 \rightarrow \underset{\text{EO}}{C_2H_4O} \qquad \zeta_1 \tag{2}$$

$$\underset{\text{ethylene}}{C_2H_4} + 3O_2 \rightarrow 2CO_2 + 2H_2O \tag{3}$$

$$\underset{\text{EO}}{C_2H_4O} + 2.5O_2 \rightarrow 2CO_2 + 2H_2O \qquad \zeta_2 \tag{4}$$

where ζ_i is the extent of reaction *i*.

For this project, it may be assumed that the second reaction, Equation (3), does not occur to any appreciable extent.

Based on the catalyst and reaction kinetics, the reactor must operate between 25-35 bar. The reactor operates isothermally at 240°C. Since the reaction is exothermic, a medium is needed to remove the heat generated, and that medium must always be at a lower temperature than that of the reactor.

Table 1 shows the selectivity data for the reactions as a function of conversion. The conversion in the reactor should be one decision variable.

Table 1: Reaction Selectivity Data

% Conversion	ζ_1 / ζ_2
20	6.0
30	5.9
40	5.8
50	5.6
60	5.2
70	4.4
80	3.6
85	2.4
90	1.2
95	0.0

Heat Exchanger (E-702):

This unit cools and partially condenses the reactor effluent to 45°C.

Absorber (T-701):

In this absorber, water is used to remove the ethylene oxide from the other components in the gas phase. For this project only, you may assume that all of the ethylene oxide is removed, that no water is lost to the gas phase, and that no gases other than ethylene oxide are removed from the gas phase. The molar ratio of water to ethylene oxide content of Stream 8 is 100/1.

Distillation Column (T-702):

This distillation column separates EO from water. The temperature of the distillate is the temperature at which EO condenses at the column pressure of 10 bar. The valve before the distillation column reduces the pressure from 30 bar to 10 bar.

Heat Exchanger (E-703):

In this heat exchanger, the contents of the top of T-702 (pure EO) are condensed from saturated vapor to saturated liquid at the column pressure at a rate three times the flow of Stream 14. One-third of the condensate becomes Stream 14 and the remainder is returned to the column. There is a cost for the amount of cooling medium needed to remove the necessary energy. The cooling medium must always be at a lower temperature than the stream being condensed.

Heat Exchanger (E-704):

In this heat exchanger, you may assume that the stream being vaporized has the same flowrate as Stream 15. The stream is vaporized from saturated liquid to saturated vapor at the column pressure and is returned to the column. The temperature of the stream being vaporized is the boiling point of water at the column pressure. There is a cost for the amount of steam needed to supply the necessary heat. The steam temperature must be above the temperature of the vaporizing stream.

Other Equipment:

For two or more streams to mix, they must be at identical pressures. Pressure reduction may be accomplished by adding a valve. All of these valves are not necessarily shown on the attached flowsheet, and it may be assumed that additional valves can be added as needed at no cost. Flow occurs from higher pressure to lower pressure. Pumps increase the pressure of liquid streams, and compressors increase the pressure of gas streams.

Additional Information:

If you make steam from boiler feed water anywhere in the process, you may take credit for the value of all steam produced minus the cost of boiler feed water. A pump will also be needed to raise the pressure of boiler feed water to that of the steam produced.

Design of Heat Exchangers E-701 and E-702

A detailed design of E-701 and E-702 is required for base-case conditions. It should be assumed that cooling water and other utilities are available at the conditions specified in the Appendix of this problem statement. For this heat exchanger design, the following information should be provided:

- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Diameter, tube-wall thickness, shell-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the two exchangers should be included along with a set of comprehensive calculations in an appendix for the design of the heat exchangers. You should use ASPEN Exchanger Design & Rating (EDR) in the ASPEN Plus simulator to carry out the detailed design.

Economic Analysis

When evaluating alternative cases, you should carry out an economic evaluation and profitability analysis based on a number of economic criteria such as payback period, internal rate of return, and cash flow analysis. In addition, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

EAOC = – (product value – feed cost – other operating costs – capital cost annuity)

A negative EAOC means there is a profit. It is desirable to minimize the EAOC; i.e., a large negative EAOC is very desirable, although you are **not** being asked to carry out optimization.

The costs for EO and ethylene (highest purity) can be found in the *Chemical Market Reporter*. The cost for "pure" oxygen is \$0.20/100 std ft^3 (60°F, 1 atm).

Other operating costs are utilities, such as steam, cooling water, natural gas, and electricity.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed cost of plant construction. The capital cost annuity is defined as follows:

$$\textit{capital cost annuity} = FCI \frac{i(1+i)^n}{(1+i)^n - 1}$$

where *FCI* is the installed cost of all equipment; *i* is the interest rate, $i = 0.15$; and *n* is the plant life for accounting purposes, $n = 10$.

For detailed sizing, costing, and economic evaluation including profitability analysis, you may use the Aspen Process Economic Analyzer (formerly Aspen Icarus Process Evaluator) in Aspen Plus Version 8. However, it is also a good idea to independently verify the final numbers based on other sources such as cost data given below.

Other Information

You should assume that a year equals 8,000 hours. This is about 330 days, which allows for periodic shut-down and maintenance.

Final Comments

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. You may need to fill in some missing data by doing a literature search, Internets search, or making assumptions. The possibility exists that as you work on this problem, your questions will require revisions and/or clarifications of the problem statement. You should be aware that these revisions/clarifications may be forthcoming.

Moreover, in some areas (e.g. sizing/costing) you are given more data and information than what is needed. You must exercise engineering judgment and decide what data to use. Also you should also seek additional data from the literature or Internet to verify some of the data, e.g. the prices of products and raw materials.

References

1. Felder, R. M. and R. W. Rousseau, *Elementary Principles of Chemical Processes (3rd ed.)*, Wiley, New York, 2000.

2. Perry, R. H. and D. Green, eds., *Perry's Chemical Engineering Handbook (7th ed.)*, McGraw-Hill, New York, 1997.

Appendix 1

Reaction Kinetics

The pertinent reactions are as follows:

$$C_2H_4 + 0.5\,O_2 \rightarrow C_2H_4O \tag{1}$$

$$C_2H_4 + 3\,O_2 \rightarrow 2CO_2 + 2H_2O \tag{2}$$

$$C_2H_4O + 2.5\,O_2 \rightarrow 2CO_2 + 2H_2O \tag{3}$$

The kinetic expressions are, respectively:

$$r_1 = \frac{1.96\exp(-2400/RT)\,p_{ethylene}}{1 + 0.00098\exp(11200/RT)\,p_{ethylene}} \tag{4}$$

$$r_2 = \frac{0.0936\exp(-6400/RT)\,p_{ethylene}}{1 + 0.00098\exp(11200/RT)\,p_{ethylene}} \tag{5}$$

$$r_3 = \frac{0.42768\exp(-6200/RT)\,p^2_{ethylene\ oxide}}{1 + 0.000033\exp(21200/RT)\,p^2_{ethylene\ oxide}} \tag{6}$$

The units for the reaction rates are moles/m^3 s. The pressure unit is bar. The activation energy numerator is in cal/mol.

Other data:

catalyst: silver on inert support, spherical catalyst support, 7.5 mm diameter
bulk catalyst density = 1250 kg/m^3
void fraction = 0.4

Appendix 2

Economic Data

Equipment Costs (Purchased)

Pumps	\$630(power, kW)$^{0.4}$
Heat Exchangers	\$1030(area, m^2)$^{0.6}$
Compressors	\$770(power, kW)$^{0.96}$ + 400(power, kW)$^{0.6}$
Turbine	\$2.18×10^5(power output, MW)$^{0.6}$ assume 65% efficiency
Fired Heater	\$635(duty, kW)$^{0.8}$ assume 80% thermal efficiency assume can be designed to use any organic compound as a fuel
Vessels	\$$[1.67(0.959 + 0.041P - 8.3\times10^{-6}P^2)]\times10^z$ $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$ D = diameter, m $0.3 \text{ m} < D < 4.0 \text{ m}$ L = height, m $L/D < 20$ P = absolute pressure, bar
Catalyst	\$2.25/kg
Packed Tower	Cost as vessel plus cost of packing
Packing	\$$(-110 + 675D + 338D^2)H^{0.97}$ D = vessel diameter, m; H = vessel height, m
Tray Tower	Cost as vessel plus cost of trays
Trays	\$$(187 + 20D + 61.5D^2)$ D = vessel diameter, m
Storage Tank	\$$1000V^{0.6}$ V = volume, m^3
Reactors	isothermal packed bed reactor cost = \$2.25×10^4[heat transfer area (m^3)]$^{0.5}$ cooling fluid in shell and catalyst in tubes adiabatic packed bed reactor cost = \$4.57×10^4[volume of reactor (m^3)]$^{0.67}$ does not include cost of subsequent heat exchangers The "volume of reactor" includes the catalyst plus the void volumes.

It may be assumed that pipes and valves are included in the equipment cost factors. Location of key valves should be specified on the PFD.

Raw Materials and Products

See *Chemical Market Reporter*

Oxygen from cryogenic plant	\$0.20/100 std ft^3 (60°F, 1 atm).

Utility Costs

Low Pressure Steam (618 kPa saturated)	\$7.78/1000 kg
Medium Pressure Steam (1135 kPa saturated)	\$8.22/1000 kg
High Pressure Steam (4237 kPa saturated)	\$9.83/1000 kg
Natural Gas (446 kPa, 25°C)	\$6.00/GJ
Fuel Gas Credit	\$5.00/GJ
Electricity	\$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	\$2.45/1000 kg
Cooling Water available at 516 kPa and 30°C return pressure ≥ 308 kPa return temperature is no more than 15°C above the inlet temperature	\$0.354/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ≥ 308 kPa return temperature is no higher than 20°C	\$4.43/GJ
Deionized Water available at 5 bar and 30°C	\$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit
Refrigeration	\$7.89/GJ
Wastewater Treatment	\$56/1000 m^3

Any fuel gas purge may be assumed to be burned elsewhere in the plant at a credit of \$2.50/GJ. It may also be assumed that all steam produced can be returned to the steam supply system for the appropriate credit. Steam produced and returned to the steam supply system must be provided at one of the usual pressure levels. For all steam produced that is returned as condensate, there is no cost for boiler feed water.

Equipment Cost Factors

Total Installed Cost = Purchased Cost (4 + material factor (MF) + pressure factor (PF))

Pressure < 10 atm, PF = 0.0	does not apply to turbines, compressors, vessels,
(absolute) 10 - 20 atm, PF = 0.6	packing, trays, or catalyst, since their cost
20 - 40 atm, PF = 3.0	equations include pressure effects
40 - 50 atm, PR = 5.0	
50 - 100 atm, PF = 10	

Carbon Steel	MF = 0.0
Stainless Steel	MF = 4.0

Appendix 3

Other Design Data

Heat Exchangers

For heat exchangers, use the following approximations for heat-transfer coefficients to allow you to determine the heat transfer area:

situation	h (W/m^2°C)
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	1000
flowing liquid	600
flowing gas	60