Separations and Reaction Engineering

Design Project

Ethylene Oxide Production

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 120,000 tonne/y of ethylene oxide in an 8000-hour year.

Process Description

One possible process flow diagram is shown in Figure 1. You may use this as a base case. However, it is part of this design assignment for you to optimize this process configuration. It is almost certain that this is not the optimum process configuration. Ethylene feed (via pipeline from a neighboring plant) is mixed with recycled ethylene and mixed with compressed and dried air (drying step not shown), heated, and then fed to the first reactor. The reaction is exothermic, and medium-pressure steam is made in the reactor shell. Conversion in the reactor is kept low to enhance selectivity for the desired product. The reactor effluent is cooled, compressed, and sent to a scrubber where ethylene oxide is absorbed by water. The vapor from the scrubber is heated, throttled, and sent to a second reactor, followed by a second series of cooling, compression, and scrubbing. The optimum number of reactor-absorbers is unclear. A fraction of the unreacted vapor stream is purged with the remainder recycled. The combined aqueous product streams are mixed, cooled, throttled, and distilled to produce the desired product. The required purity specification is 99.5 wt% ethylene oxide.

Feed Conditions

The feed ethylene is available at 50 bar and 25°C. The feed air is available at 1 atm and 25°C. Oxygen from a cryogenic plant is available at 1 atm and 25°C. If air is used, there must be sufficient excess air so that the ethylene is below its LFL of 3.1 vol%. If purified oxygen is used, the oxygen/ethylene ratio should be identical to that in the air case. For pure oxygen (99 wt% – remainder assumed to be nitrogen), you may assume that a cryogenic process can be built nearby that produces oxygen.

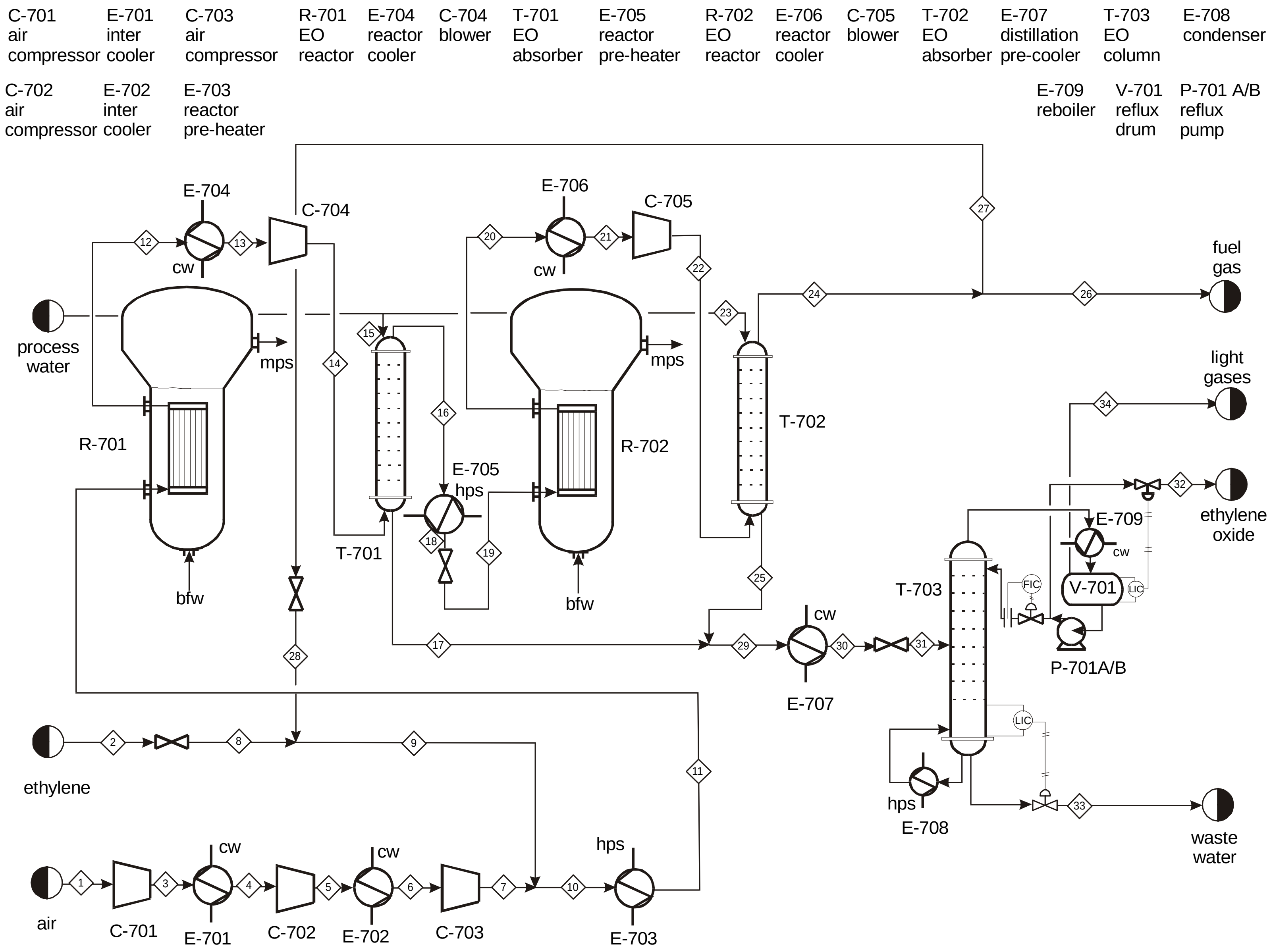

Figure 1: Process Flow Diagram for Ethylene Oxide Production

Specific Assignments

ChE 312

Determine the number of absorbers and distillation columns required, their locations, and enough information for each column to determine their costs. For the absorbers, this requires that a choice between packed and tray towers be made. The distillation column that purifies the ethylene oxide should be designed in detail. A detailed design of a tray tower includes number of trays, tray spacing, diameter, reflux ratio, active area, weir height, top and bottom pressure specifications, and design of auxiliary equipment (heat exchangers, pump, reflux drum, if present). A detailed design of a packed tower includes height, packing size and type, and the same other specifications as in a tray tower. For all columns in this project, you may assume that HETP = 1.5 m. For the distillation column, the better economical choice between a packed and tray tower should be determined. For either a packed or a tray distillation column, the optimum reflux ratio should be determined.

Note that a tower consists of a vessel with internals (trays or packing). The constraints on a vessel are typically a height-to-diameter ratio less than 20. However, it is possible to extend this ratio to 30 as long as the tower is less than about 3 ft (1 m) in diameter. For larger-diameter towers, stresses caused by wind limit the actual height. Extra supports are needed for a height-to-diameter ratio above 20, even for smaller diameter columns. Therefore, there is a capital cost “penalty” of an additional 25% (only on the vessel) up to a ratio of 25, and a “penalty” of an additional 100% up to a ratio of 30.

ChE 325

Two reactor types may be considered for use in this design. They are an adiabatic packed-bed reactor and an “isothermal” packed bed reactor. An “isothermal” packed-bed reactor is defined here as one with a specified outlet temperature. The temperature along the length of the packed-bed reactor is not constant. The temperature can be controlled by varying the temperature and flowrate of the heat-transfer fluid, heat-transfer area, and the catalyst/inert ratio. One suggestion for the heat-transfer fluid is Dowtherm™ A; however, you may make another choice, such as making steam from boiler feed water or using cooling water. If a heat-transfer fluid is used, it is circulated in a closed loop through the reactor where its temperature is increased. Then, heat is removed from the fluid in a heat exchanger. The cooled heat-transfer fluid is then pumped back to the reactor.

For your best case, you should include a discussion of the temperature, pressure, and concentration profiles obtained from Chemcad.

General

The entire ethylene oxide process should be optimized using decision variables of your choosing. Decision variables should be chosen as the design variables most strongly affecting the objective function. There are topological optimization and parametric optimization. In topological optimization, which is usually done first, the best process configuration is to be chosen. Some suggested choices (but not the only possible choices) include using oxygen vs. of air, the number of compressor stages, whether or not to use refrigerated water for intercooling the compressor stages, the type of reactor, the method of heat removal in an "isothermal" reactor, the number of reactor-absorber stages, whether to refrigerate the process water used in the absorbers, and the location of heat exchangers, etc. Parametric optimization involves varying operating variables and should be done after topological optimization is complete. Examples of parameters that can be used as decision variables are reactor temperature, pressure, and conversion; absorber temperature and pressure; and distillation column reflux ratio.

Economic Analysis

When evaluating alternative cases, the equivalent annual operating cost (EAOC) objective function should be used. The EAOC is defined as

EAOC = -(product value - feed cost – utility costs – waste treatment cost - 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.

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:

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

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

Report Format

This report should conform to the Department guidelines. It should be bound in a folder that is not oversized relative to the number of pages in the report. Figures and tables should be included as appropriate. An appendix should be attached that includes sample calculations. These calculations should be easy to follow.

The written report is a very important part of the assignment. Poorly written and/or organized written reports may require re-writing. Be sure to follow the format outlined in the guidelines for written reports. Failure to follow the prescribed format may be grounds for a re-write.

The following information, at a minimum, must appear in the main body of the final report:

1. a computer-generated PFD (not a Chemcad PFD) for the recommended optimum case,

2. a stream table containing the usual items,

3. a list of new equipment for the process, including bare module and installed costs, plus equipment specifications (presented with a reasonable number of significant figures),

4. a summary table of all utilities used,

5. a clear summary of alternatives considered and a discussion, supported with figures, of why the chosen alternative is superior,

6. a clear economic analysis which justifies the recommended case

7. a discussion section pertinent to each class plus a general discussion section for optimization of the entire process

8. a Chemcad report only for your optimized case (in the Appendix). This must contain the equipment connectivity thermodynamics, and overall material balance cover pages, stream flows, equipment summaries, tower profiles, and tray (packing) design specifications (if you use Chemcad to design the trays (packing)). It should not contain stream properties. Missing Chemcad output will not be requested; credit will be deducted as if the information is missing.

Other Information

Unless specifically stated in class, the information in this document is valid for this project only. Any information in the sophomore projects not specifically stated in this document is not valid for this project.

Deliverables

Each group must deliver a report (two identical copies, one for each professor) written using a word processor. The report should be clear and concise. The format is explained in the document *Written Design Reports*. Any report not containing a labeled PFD and a stream table, each in the appropriate format, will be considered unacceptable. PFDs from Chemcad are generally unsuitable unless you modify them significantly. When presenting results for different cases, graphs are superior to tables. For the optimal case, the report appendix should contain details of calculations that are easy to follow. There should be separate appendices for each class, ChE 312 and ChE 325, each containing calculations appropriate for the respective class. These may be handwritten if done so neatly. Calculations that cannot be easily followed will lose credit.

Each group will give an oral report in which the results of this project will be presented in a concise manner. The oral report should be between 15-20 minutes, and each group member must speak once. Reports exceeding this time limit will be stopped. A 5-10 minute question-and-answer session will follow. Instructions for presentation of oral reports are provided in a separate document entitled *Oral Reports*. The oral presentations will be Wednesday, April 23, 2003, starting at 11:00 a.m. and running until approximately 3:00 p.m. Attendance is required of all students during their classmates' presentations (this means in the room, not in the hall or the computer room). Failure to attend any of the above-required sessions will result in a decrease of one letter grade (per occurrence) from your project grade in ChE 312 and ChE 325.

The written project report is due by 11:00 a.m. Wednesday, April 23, 2003. Late projects will receive a minimum deduction of one letter grade.

In order to evaluate each team members writing skills, the results and discussion sections for each specific assignment should be written by a different team member. The authorship of each of these specific assignments should be clearly specified in the report. If a team has four members, the member not authoring a specific assignment should author the introduction and conclusion.

Revisions

As with any open-ended problem (*i.e.*, a problem with no single correct answer), the problem statement above is deliberately vague. 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.

Appendix 1
Reaction Kinetics

The pertinent reactions are as follows:

$$C_2H_4 + 0.5\,O_2 \rightarrow C_2H_4O \qquad (1)$$

$$C_2H_4 + 3\,O_2 \rightarrow 2CO_2 + 2H_2O \qquad (2)$$

$$C_2H_4O + 2.5\,O_2 \rightarrow 2CO_2 + 2H_2O \qquad (3)$$

The kinetic expressions are, respectively:

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

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

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

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
Chemcad Instructions

For Chemcad simulations, the following thermodynamics packages are ***strongly*** recommended for simulation of this process:

K-values:	global – PSRK; local for absorbers – Unifac
enthalpy:	SRK

It is recommended that you begin to simulate the process without recycle and add needed recycle streams after you have successfully simulated each unit. Since towers can be difficult to converge, it is acceptable to use a shortcut column in the simulation including recycle, and have a TOWR or a SCDS as a separate unit, removed from the process including recycle. You can copy the shortcut feed stream as the feed stream of the new unit. However, be aware that each time you change the process and re-simulate it, the stream must be recopied and the individual unit re-run; it does not copy and run automatically.

There will be some light, non-condensable gases remaining in the feed to the distillation column. Their presence makes simulation of the distillation column difficult. Therefore, for simulation purposes, you may add a component separator before the distillation column to remove these components, leaving only ethylene oxide and water entering the distillation column. This stream comprises the light-gas purge stream from the reflux drum. However, the “fake” separator is a Chemcad trick, and it must not appear on any process flow diagram.

Appendix 3
Other Process Information

Because the PFD in Figure 1 is so crowded, some items that are present in the actual process have been deliberately omitted. These are:

1. the direction of the process flow in the reactors. In Figure 1, it is shown as being upward to avoid too many line crosses. It is actually downward.

2. the pump(s) for the boiler feed water feed to the reactors. The pumps take boiler feed water at 90°C and 550 kPa and raise the pressure to that required to make steam. The cost of this pump(s) should be included in the economic analysis.

3. the pump(s) for process water. The pump takes process water at 5 bar and 30°C and raises the pressure to the required feed pressure to the scrubbers. The cost of this pum(s) should be included in the economic analysis.

If you use the process in Figure 1 as a base case, the following values may be used in that base case:

pressure of reactor feeds	26.5 bar
temperature of reactor feeds	240°C
conversion in each reactor of limiting reactant	20%
pressure of absorbers	30 bar
temperature of process stream inlet to absorbers	64°C
pressure of distillation column	10 bar

Appendix 4
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 (absolute)	< 10 atm, PF = 0.0 10 - 20 atm, PF = 0.6 20 - 40 atm, PF = 3.0 40 - 50 atm, PR = 5.0 50 - 100 atm, PF = 10	does not apply to turbines, compressors, vessels, packing, trays, or catalyst, since their cost equations include pressure effects

Carbon Steel	MF = 0.0
Stainless Steel	MF = 4.0

Appendix 5
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/m²°C)
condensing steam	6000
condensing organic	1000
boiling water	7500
boiling organic	1000
flowing liquid	600
flowing gas	60

Physical Properties of Dowtherm™ A

temperature use range (in liquid phase)	60°F – 750°F
vapor pressure at 750°F	137.8 psig
thermal conductivity (avg. over use range)	0.07 BTU/hr ft°F
heat capacity (avg. over use range)	0.5 BTU/lb°F
viscosity (at max. and min. temp. use range)	0.14 cp, 6.0 cp
density (avg. over use range)	54 lb/ft^3