Energy Balances and Numerical Methods
Spring 2002

Design Project

Production of Ethylene Oxide

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/y.

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 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/y, may be assumed pure

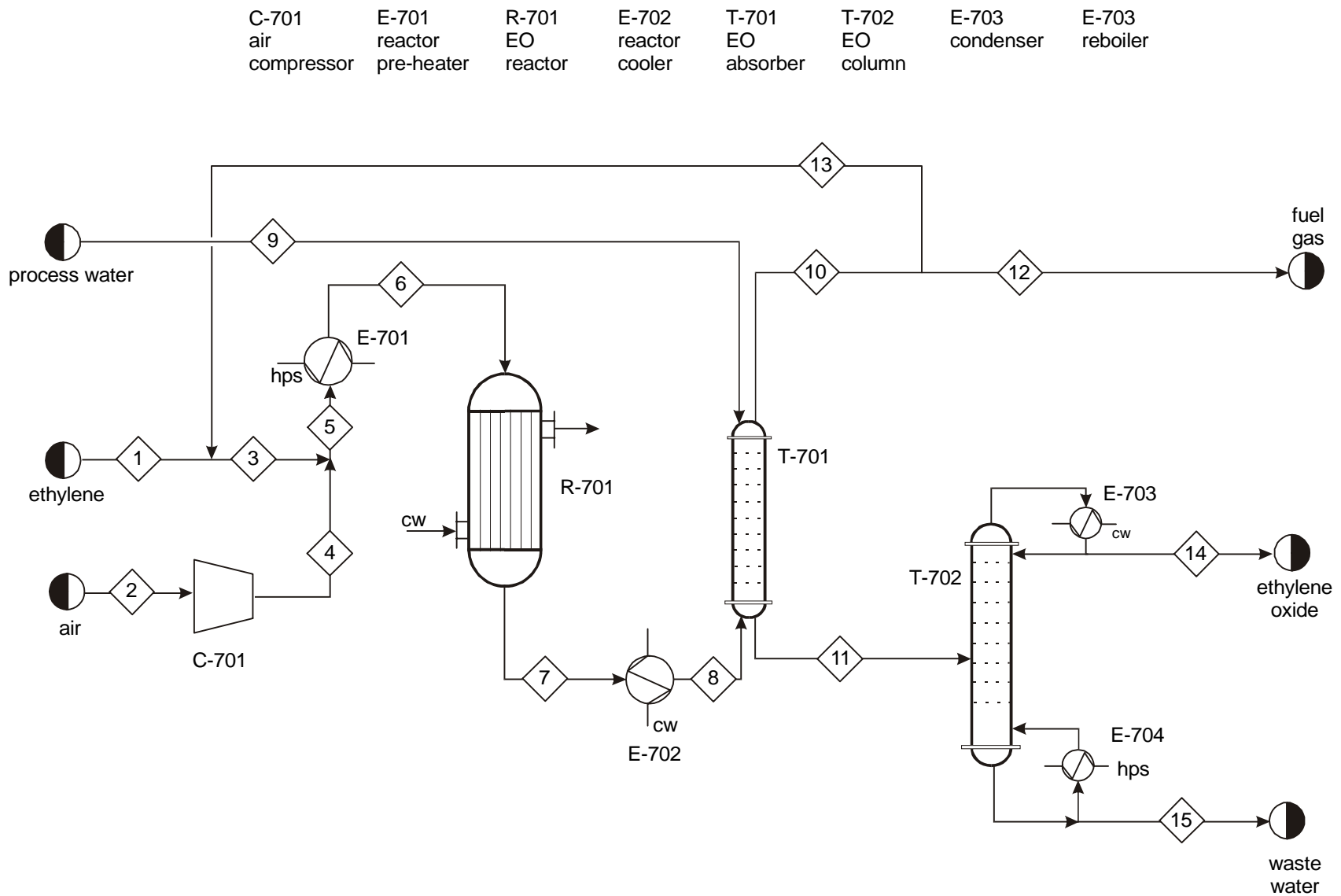| C-701 | E-701 | R-701 | E-702 | T-701 | T-702 | E-703 | E-703 |
| air compressor | reactor pre-heater | EO reactor | reactor cooler | EO absorber | EO column | condenser | reboiler |

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

$$W_s = 4.5RT_{in}\left[\left(\frac{P_{out}}{P_{in}}\right)^{0.286} - 1\right] \tag{1}$$
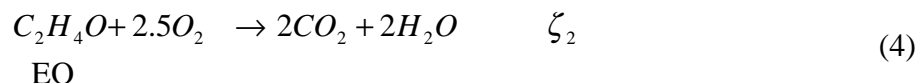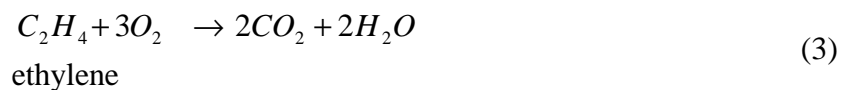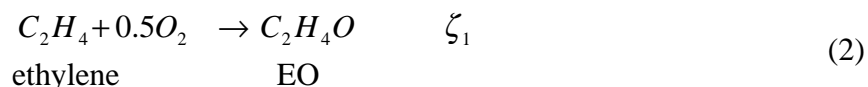
where the work is in kJ/kmol and the temperature is in Kelvin.

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:

$$\begin{array}{cc} C_2H_4 + 0.5O_2 & \rightarrow C_2H_4O \qquad \zeta_1 \\ \text{ethylene} & \text{EO} \end{array} \tag{2}$$

$$\begin{array}{c} C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O \\ \text{ethylene} \end{array} \tag{3}$$

$$\begin{array}{cc} C_2H_4O + 2.5O_2 & \rightarrow 2CO_2 + 2H_2O \qquad \zeta_2 \\ \text{EO} \end{array} \tag{4}$$

where ζ_i is the extent of reaction i.

For this semester, 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 semester's 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. For this semester only, the separation may be assumed to be perfect, i.e., pure EO is produced in the distillate. 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.

Utility Costs

Low-Pressure Steam (618 kPa, saturated, cost or credit) $6.62/1000 kg

Medium-Pressure Steam (1135 kPa, saturated, cost or credit) $7.31/1000 kg

High-Pressure Steam (4237 kPa, saturated, cost or credit) $8.65/1000 kg

Natural Gas or Fuel Gas (446 kPa, 25°C)
     cost $3.00/GJ
     credit $2.50/GJ

Electricity $0.05/kWh

Boiler Feed Water (at 549 kPa, 90°C) $2.54/1000 kg
(There is only a cost for boiler feed water if the steam produced enters process streams. If it is condensed, it can be made into steam again, so there is no net cost for boiler feed water.)

Cooling Water $0.16/GJ
     available at 516 kPa and 30°C
     return pressure ≥ 308 kPa
     return temperature should be no more than 15°C above the inlet temperature

Refrigerated Water $20/GJ
     available at 516 kPa and 5°C
     return pressure ≥ 308 kPa
     return temperature is no higher than 15°C

Process Water $0.04/1000 kg
     available at 300 kPa and 25°C

Waste Water Treatment $50/1000 m^3

Data

Use data from in Felder and Rousseau[1] or from any handbook[2]. The following data are not readily available in these references.

Liquid Heat Capacity
for EO: $144{,}710 - 758.87T + 2.8261T^2 - 0.003064T^3$ J/kmol K T (K)

Vapor Heat Capacity
for EO: $33{,}460 + 121{,}160\left[\dfrac{1608.4/T}{\sinh(1608.4/T)}\right]^2 + 82{,}410\left[\dfrac{737.3/T}{\cosh(737.3/T)}\right]^2$ J/kmol K T (K)

Normal Heat of Vaporization
for EO: 30,348 J/mol

Heat of Formation
for EO: -1194.7 kJ/kg

Vapor Pressure
for EO: $\ln P^*(\text{Pa}) = 91.949 - 5293.4/T - 11.682 \ln T + 0.014913T$ T(K)

Economic Analysis

When evaluating alternative cases, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and 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 costs for EO and ethylene (highest purity) can be found in the *Chemical Market Reporter*, which is in the Evansdale Library. 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. A list of capital costs for all pieces of equipment will be provided in early to mid March.

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, $i = 0.15$; and n is the plant life for accounting purposes, $n = 10$.

Optimization

We will learn optimization methods in ChE 230. The objective function (EAOC) is defined above. It is your responsibility to define appropriate decision variables. If there are too many decision variables to do a reasonable optimization, it is your responsibility to determine, with appropriate justification, which ones most significantly affect the objective function and focus on only those decision variables.

Other Information

You should assume that a year equals 8000 hours. This is about 330 days, which allows for periodic shut-down and maintenance.

Deliverables

Each group must deliver a report written using a word processor. The report should be clear and concise. The format is explained in a separate document (*Written Design Reports*). Any report not containing a labeled PFD and a stream table will be considered unacceptable. The stream table must include temperature, pressure, phase, total mass flowrate, total molar flowrate, and component molar flowrates. When presenting results for different cases, graphs are generally superior to tables. The report appendix should contain details of calculations for the optimal case. These calculations may be (neatly) hand-written. **Calculations that can not be followed easily will lose credit.** (If you are in doubt as to the meaning of this statement, ask the instructor.) Refer to the document entitled *Written Design Reports* for more information.

Each group will give an oral report in which the results of this project are presented in a concise manner. The oral report should be no more than 15 minutes, and each group member must speak. A 5-10 minute question-and-answer session will follow. Instructions for presentation of oral reports will be provided in a separate document entitled *Oral Reports*. However, the best way to learn how to present an oral report, other than actually presenting one, is to make time to see some of the oral reports presented by the juniors the week before you are to present your report. The presentations will most likely be on Wednesday, April 24, 2002, between 11:00 a.m. and 3:00 p.m. You will be kept informed of the scheduling of these presentations.

As mentioned in the cover memo, the written project report is due on Monday, April 29, 2002, at 3:00 p.m. The oral reports will be Monday, April 29, 2002 and Wednesday, May 1, 2002 (ChE 230 classes). There will be a project review on Thursday, May 2, 2002 (ChE 202 class). In addition, everyone must attend the senior design presentation at 2:30 pm on Tuesday, April 30, 2002. Furthermore, 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 in one letter grade (per occurrence) from your project grade in both ChE 202 and ChE 230.

Anyone not participating in this project will automatically receive an F for ChE 202 and ChE 230, regardless of other grades earned in this classes.

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.

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.

MEMORANDUM

TO: Sophomores in ChE 202 and ChE 230

FROM: R. K. Gupta
             C. D. Stinespring

DATE: May 7, 2002

SUBJECT: Equipment Costs for Design Project

   The equipment costs for the ethylene oxide plant are given below. Each cost is for an individual piece of equipment, including installation.

Equipment	Installed Cost in millions of $
Reactor	10
Distillation Columns, each (including peripheral heat exchangers)	2.5
Absorber	5
Compressor	$0.24 \times (\text{flow, kmol/h})^{0.6}$
Heat Exchangers, all, including ones not shown on process flow diagram	13

For the compressor, flow is the total molar flowrate through the compressor

Fired Heater installed cost in dollars:
$$11 \times 10^{x}$$
where
$$x = 2.5 + 0.8 \log_{10} Q$$
where Q is the heat duty in kW