

**ChE 456**  
**Spring 2002**  
**Major 2**

**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 in the pacific basin. Your assignment is to design a new, grass-roots facility to produce 120,000 tonne/y of ethylene oxide in an 8000-hour year.

**Alternatives**

You are free to optimize using any process alternatives you believe to be reasonable. At a minimum, you should consider the use of air (assumed to be 79 wt% nitrogen and 21 wt% oxygen) as the source of oxygen vs. the use of purified oxygen. You should also consider adiabatic vs. isothermal reactors. For isothermal reactors, you might also consider alternative methods for heat removal.

**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. There must be sufficient excess air or oxygen 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.

**Economics**

For the new process, use a 10%, after-tax rate of return and a 10-year lifetime after start-up. Use the 5-year MACRS depreciation method. Assume that there is a two-year construction period, with 60% of the capital cost paid after the first year and 40% paid after the second year. The land cost is \$1 million, paid at the beginning of the project (end of year 0). Six months of working capital (based on  $COM_d$ ) is needed at the beginning of production. There is no salvage value for the equipment. The taxation rate is 30%. (There are lower tax rates in the pacific basin.)

You should use the utility costs in Table 3.4 of the textbook. Note that the cost of cooling water, refrigerated water, etc., is based on the energy usage, not the return temperature. The

maximum return temperature for cooling water is 45°C. Refrigerated water it is available at 5°C with a maximum return temperature of 15°C, and its cost is \$20/GJ.

The prices for ethylene (highest grade possible) and ethylene oxide are available in the *Chemical Market Reporter*. For pure oxygen (99 wt% – remainder assumed to be nitrogen), you may assume that a cryogenic process can be built nearby that produces oxygen at a cost of \$0.20/100 std ft<sup>3</sup> (60°F, 1 atm).

The fixed capital investment for this process should be based on the grass-roots facility cost given by CAPCOST.

The capital costs for reactors are not included in CAPCOST. These may be entered as “user added equipment.” The following cost estimates are bare module costs for different reactor types:

$$\text{fluidized bed reactor cost} = \$2.29 \times 10^5 [\text{volume of reactor (m}^3\text{)}]^{0.67}$$

$$\text{packed bed reactor cost} = \$2.25 \times 10^4 [\text{heat transfer area (m}^2\text{)}]^{0.5}$$

cooling fluid in shell and catalyst in tubes

$$\text{packed bed reactor cost} = \$4.57 \times 10^4 [\text{volume of reactor (m}^3\text{)}]^{0.67}$$

does not include cost of subsequent heat exchangers

The “volume of reactor” includes the catalyst plus the void volumes.

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.

## Deliverables

Specifically, you are to prepare the following by 9:00 am, Monday, February 18, 2002:

1. an optimized, grass-roots design for the new ethylene oxide facility,
2. a written report, conforming to the Department guidelines, detailing the design,
3. a legible, organized set of calculations justifying your recommended design, including any assumptions made,
4. a signed copy of the attached confidentiality statement.

## 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 confidentiality statement should be the very last page of the report.

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 for the recommended optimum case,
2. a stream table containing the usual items,
3. a clear summary of alternatives considered and a discussion, supported with figures, of why the chosen alternative is superior,
4. a list of new equipment for the new process, including bare module and installed costs, plus equipment specifications,
5. a summary table of all utilities used.

## Oral Presentation

You will be expected to present and defend your results some time between February 18, 2002 and February 27, 2002. Your presentation should be 15-20 minutes, followed by about a 30-minute question and answer period. Make certain that you prepare for this presentation since it is an important part of your assignment. You should bring at least one hard copy of your slides to the presentation and hand it out before beginning the presentation.

## Other Rules

You may not discuss this major with anyone, other than allowable consulting from the instructor. Discussion, collaboration, or any other interaction with anyone (including those in this class, not in this class, not at the University, on this planet, etc.) is prohibited.

Consulting is available from the instructor. Chemcad consulting, i.e., questions on how to use Chemcad, not how to interpret results, is unlimited and free, but only from the instructor. A student may receive two free minutes of consulting from the instructor. After two minutes of consulting, the rate is 2.5 points deducted for 15 minutes or any fraction of 15 minutes, on a cumulative basis. The initial 15-minute period includes the 2 minutes of free consulting.

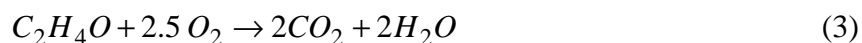
## **Late Reports**

Late reports are unacceptable. The following severe penalties will apply:

- late report on due date before noon: one letter grade (10 points)
- late report after noon on due date: two letter grades (20 points)
- late report one day late: three letter grades (30 points)
- each additional day late: 10 additional points per day

## Appendix 1 Reaction Kinetics

The pertinent reactions are as follows:



The kinetic expressions are, respectively:

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

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

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

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

These kinetic expressions are only valid in the presence of excess oxygen.

other data:

catalyst: silver on inert support, spherical catalyst support, 7.5 mm diameter

bulk catalyst density = 1250 kg/m<sup>3</sup>

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.