Fluid Mechanics, Heat Transfer, and Thermodynamics
Fall 2001

Design Project

Production of Dimethyl Ether

We are investigating the feasibility of constructing a new, grass-roots, 50,000 tonne/y, (1 tonne = 1 metric ton = 1000 kg) dimethyl ether (DME) plant. This will be part of a larger facility that also produces diethyl ether (DEE). As part of the feasibility study, we would like you to investigate some of the details of the feed and reaction sections of the proposed plant.

Dimethyl Ether Production Reaction

The primary reaction is

$$\underset{\text{methanol}}{2CH_3OH} \quad \Leftrightarrow \quad \underset{\text{dimethyl ether}}{CH_3-O-CH_3} \quad + \quad H_2O \tag{1}$$

For the purposes of this preliminary evaluation, it is assumed that the reaction occurs in an adiabatic packed bed of catalyst particles. Practical equipment limitations make the maximum possible conversion 80% of the equilibrium conversion.

Any ethanol impurity in the reactant feed reacts according to the following reactions

$$\underset{\text{ethanol}}{2C_2H_5OH} \quad \rightarrow \quad \underset{\text{diethyl ether}}{C_2H_5-O-C_2H_5} \quad + \quad H_2O \tag{2}$$

$$\underset{\text{ethanol}}{C_2H_5OH} \quad \rightarrow \quad \underset{\text{ethylene}}{C_2H_4} \quad + \quad H_2O \tag{3}$$

Feed and Reaction Sections

The PFD for the feed and reaction sections is given in Figure 1. Feed to the process consisting of liquid methanol, is mixed with recycle liquid methanol.

The reaction is equilibrium limited. Based on the catalyst and reaction kinetics, the reactor must operate at a minimum of 15 bar. The base-case reactor (inlet and outlet temperature and

P-201A/B Methanol Feed Pump	V-201 Feed Vessel	E-201 Methanol Pre-heater	R-201 Reactor	E-202 Reactor Cooler	SS Separation Section

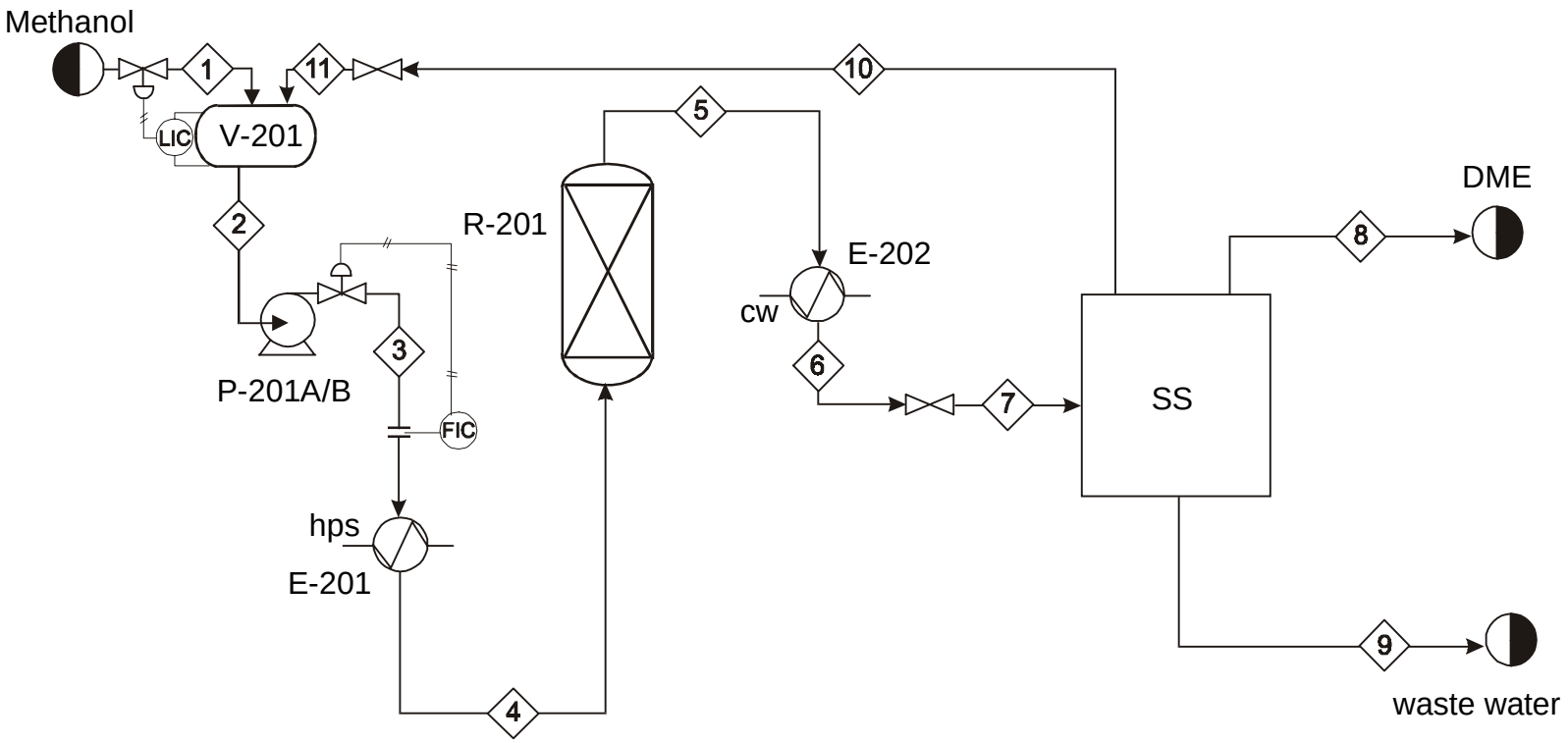


Figure 1:
Process Flow Diagram for the Feed Section for Production of Dimethyl Ether (Unit 200)

pressure) operates at the conditions of your sophomore design, *i.e.*, the optimized case. If your reactor was adiabatic, since the reaction is exothermic, the reactor effluent temperature will be above its feed temperature. If you ran the reactor isothermally, you must remember that heat removal is needed for an isothermal reactor. For an adiabatic reactor, the conversion is 80% of the equilibrium conversion at the pressure and exit temperature of the reactor.

The equilibrium expression for the reaction in Eq. (1) is

$$\ln K = -2.205 + \frac{2708.6317}{T} \tag{4}$$

where the temperature is in Kelvin.

Process Details

Feed Streams

Stream 1: methanol liquid at 110 kPa, 25°C, 99 wt% methanol, 1 wt% water

Stream 10: recycle methanol, saturated at 1200 kPa

Effluent Streams

Stream 8: DME product

Stream 9: Wastewater stream to treatment, must be at 200 kPa

Equipment Summary

V-201: Mixing Vessel – provides constant-flow feed stream to process from process stream and recycle stream, smoothes out fluctuations

E-201: Heat Exchanger – to preheat methanol feed

R-201: Reactor – either adiabatic (for the base case) or isothermal

E-202: Product cooler – outlet is saturated vapor

P-1401 A/B: Pump(s) from tank storage to V-201. (not shown on PFD – will be near tanks TK-1401 and TK-1402 – see the plot plan in Figure 2)

Assignment

The first task is to obtain base-case stream flows for the process using the conditions your group recommended in the Spring 2001 design. If your current group is a combination of multiple groups, just choose one set of results as a starting point. You may use Chemcad for this calculation, or you may use a spreadsheet. It is your choice.

The remainder of your assignment consists of four "mini-designs."

1. **Optimization of the Feed Section and Wastewater Pump.** (ChE 310) The process flow diagram is given in Figure 1. A plot plan is given in Figure 2. As you can see, the DME facility is part of a larger facility that also produces DEE. You are to size the new pump(s), P-1401 A/B (in Unit 1400 – see plot plan, pump location not actually shown). You are to determine the optimum pipe size for the piping from tank storage to V-201. The objective function for the optimization is the Equivalent Annual Operating Cost (EAOC) of the piping system including the pump ($/y). The *EAOC* is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + \text{annual operating costs for P-1401 A/B} \tag{5}$$

where *CAP* = the installed cost of P-1401 A/B and the pipe from tank storage to V-201

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{6}$$

where i = 0.15 (15% rate of return) and n = 10 (ten-year plant life).

Raw material costs should not be included, so *CAP* includes only the installed cost of pipes and pumps, and operating costs include the electricity to run the pump. Specify the liquid level to be maintained in the storage tanks to avoid cavitation of P-1401 A/B. Place the pumps, P-1401 A/B, on the ground at a location you choose. All elbows are 90°, and you should place these as needed. Indicate their location on a diagram. Pipes from the tanks to the process must follow the indicated pipe racks. We have a supply of centrifugal pumps used in other plants. Their pump curves and their NPSH curves are attached (Figure 3). We would like the flexibility for 25% scale-up in the future.

You should also do a pressure analysis of the Streams 1 through 7 to make sure all pressures balance. Valves and/or pumps must be added as needed. It may be assumed that each stream has a pressure drop of 5 kPa. Heat exchangers that are not designed may be assumed to have a pressure drop of 30 kPa, and the reactor pressure drop may be assumed to be 25 kPa. (Note: We could make you calculate this by giving you details of the packing and the size of the reactor; however, we think you already have enough to do.)

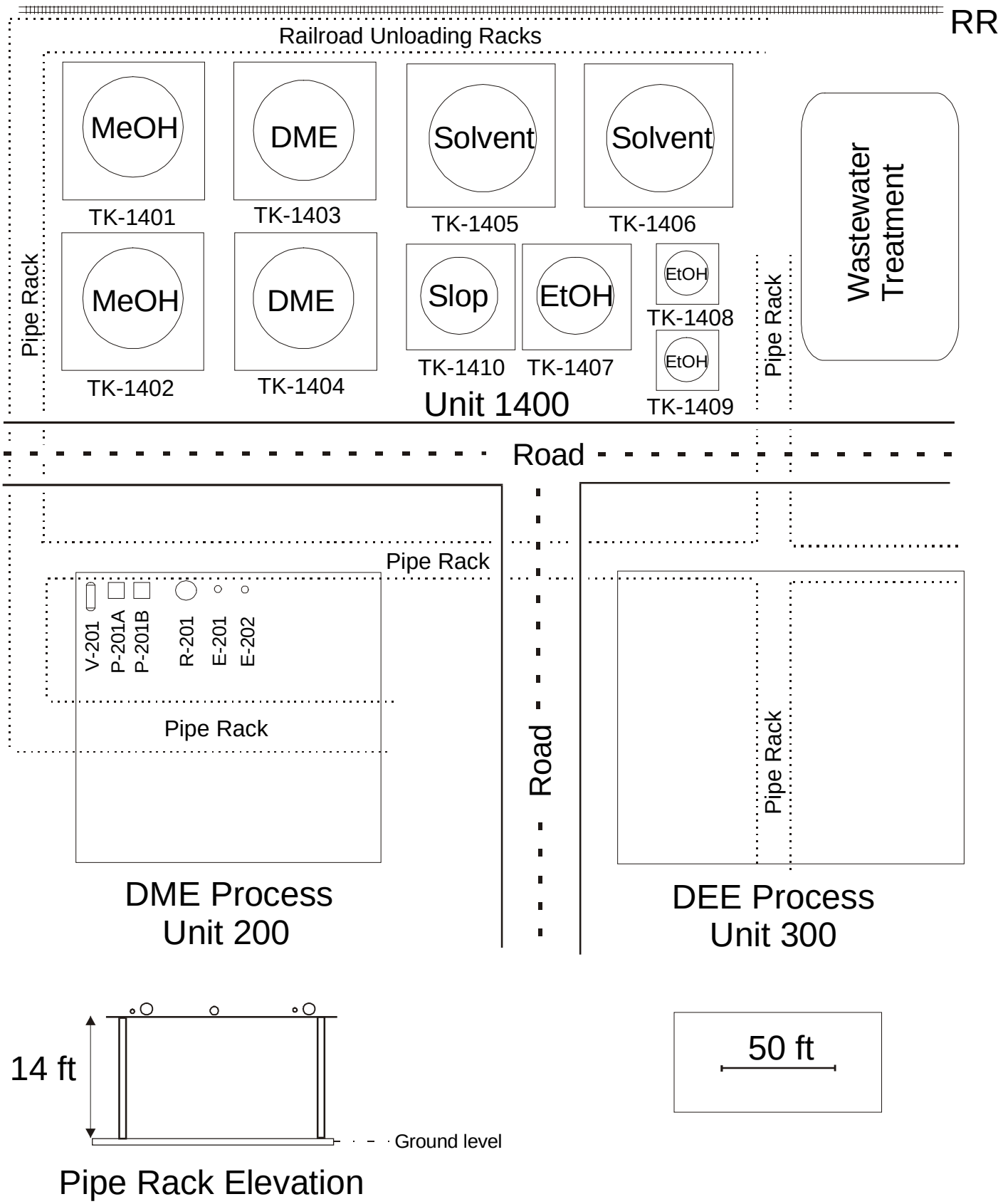
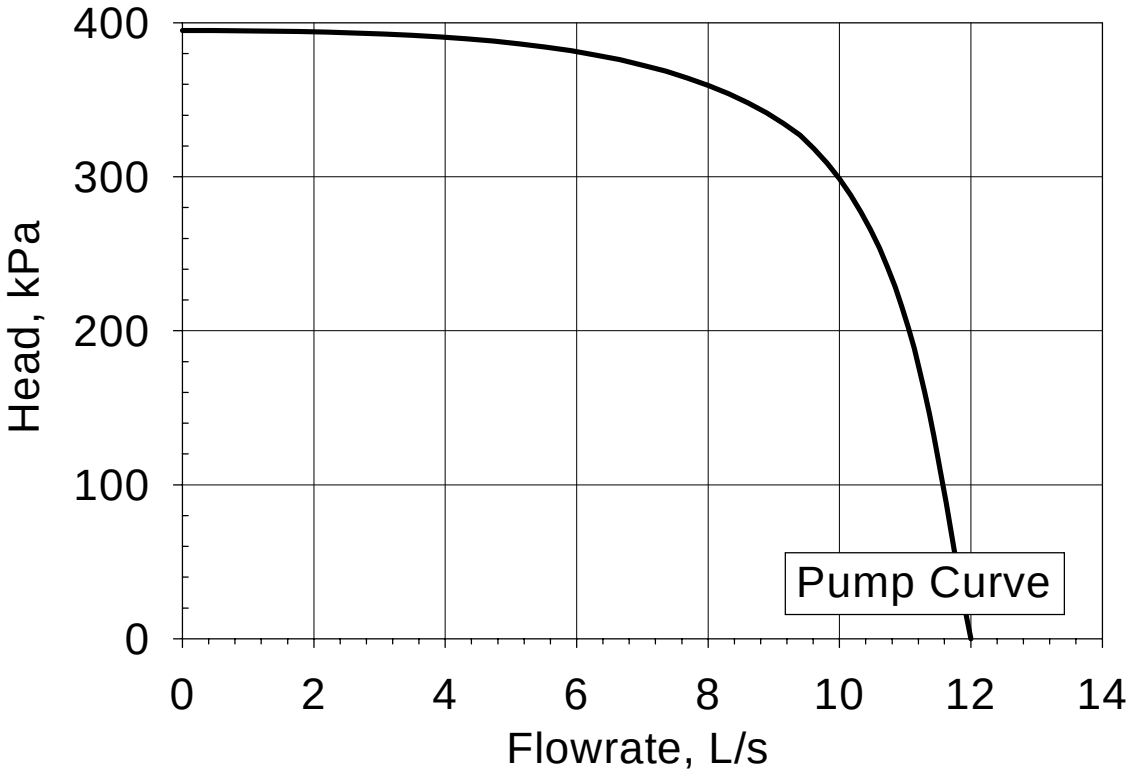


Figure 2: Plot Plan of DME/DEE Facility



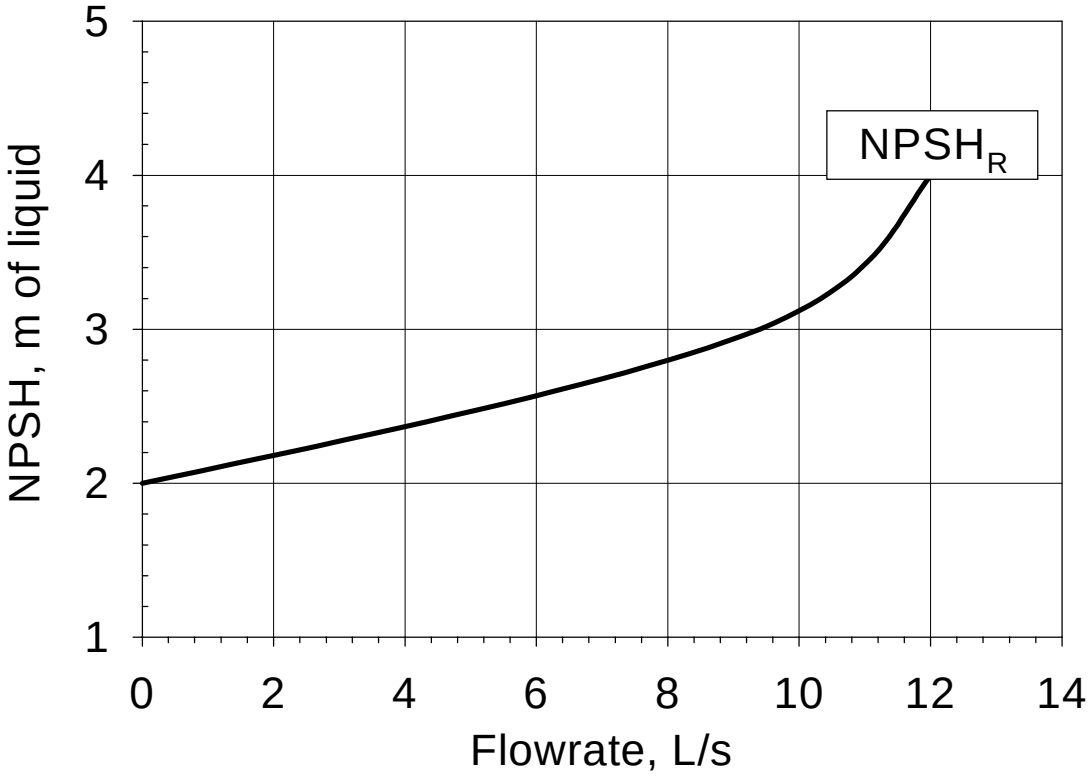


Figure 3: Pump and NPSH Curves for Pumps P-1401 A/B

2. **Design of E-202.** (ChE 311) The heat exchanger, E-202, must be designed in detail for the base case. The specifications needed for a detailed heat exchanger design will be discussed in class. The outlet pressure and temperature must be as specified, so the pressure drop of the process stream in E-202 must be consistent with the feed-section pressure analysis discussed above.

   At a minimum, you must determine the individual and overall heat transfer coefficients (including fouling factors) and the total required heat transfer area. Decide on a specific configuration for the heat exchanger, and design it in detail. Include items such as the number and length of tubes, tube-sheet layout, shell diameter, baffle spacing, tube pitch, etc. The cost of this exchanger can be calculated using the correlation given on page 10.

3. **Determination of Break-even Price (BEP) for Crude Dimethyl Ether.** (all classes) A Chemcad simulation for your base case should be presented. You should determine the BEP for crude dimethyl ether for the base case. If you choose, you may consider process modifications that improve the BEP. Full optimization is not required, but making no modifications will be considered unusual. These modifications may be in equipment and/or process conditions, such as reactor temperature, pressure, conversion, etc. The break-even price for crude dimethyl ether is calculated as follows:

$$BEP = \frac{CAP\left(\frac{A}{P}, i, n\right) + \text{cost of reactants} + \text{operating costs} - \text{byproduct revenue}}{\text{kg dimethyl ether in crude product}} \qquad (7)$$

   where *CAP* is now the installed capital cost for the entire feed and reaction sections, including the feed tanks. For this case, ignore the cost of the separation section. The crude DME product is actually the contents of Stream 7. Your discussion for this section should emphasize any differences in recommended operating conditions based on the inclusion of equipment costs and other practical matters.

4. **Thermodynamics of mixed alcohol/ether streams.** (ChE 320) We are in the process of evaluating the possibility of producing mixed ethers in a new plant using a mixed methanol/ethanol feed, with 88 mol% methanol, 11 mol% ethanol, and 1 mol% water. (In fact, you may have the opportunity to do this in the spring!) The thermodynamics of these mixtures can be very non-ideal. Therefore, you should first use Chemcad to investigate the thermodynamics of the DME-methanol-water system. Then, you should investigate the ethylene, DME, DEE, methanol, ethanol, water system. The above two lists are in order of decreasing volatility (i.e., increasing boiling point). First of all, check different thermodynamics packages in Chemcad on your base-case process to see if there are differences between the predictions of the packages. The term thermodynamics package means the choice of *K*-value and enthalpy calculation methods. At a minimum, you should investigate ideal, SRK, Peng-Robinson, NRTL, UNIQAC, UNIFAC, UNIFAC/UNIQAC. Next, examine the *T*-*x*-*y* diagrams of adjacent pairs using the same thermodynamics packages at a variety of possible operating pressures for the separation

section. The presence of azeotropes strongly affects the ability to do separations. What do you observe? Compare the predictions of the different packages.

Cost Data

Raw Materials

Methanol	see *Chemical Market Reporter*

Product

Dimethyl Ether	see *Chemical Market Reporter*

Utility Costs

Low Pressure Steam (618 kPa saturated)	$6.62/1000 kg
Medium Pressure Steam (1135 kPa saturated)	$7.31/1000 kg
High Pressure Steam (4237 kPa saturated)	$8.65/1000 kg
Natural Gas (446 kPa, 25°C)	$3.00/GJ
Fuel Gas use this price for fuel gas credit	$2.75/GJ
Electricity	$0.06/kW h
Boiler Feed Water (at 549 kPa, 90°C)	$2.54/1000 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	$0.16/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ≥ 308 kPa return temperature is no higher than 20°C	$1.60/GJ
Deionized Water available at 5 bar and 30°C	$1.00/1000 kg
Wastewater Treatment	$50/1000 m^3

Equipment Costs (Purchased)

Piping	$/m = 5.0 (diameter, in)
Valves	$100 (flow diameter, in)$^{0.8}$ for control valve with orifice plate, double the price
Pumps	$630 (power, kW)$^{0.4}$
Heat Exchangers	$1030 (area, m^2)$^{0.6}$ add 25% additional for boilers or evaporators
Compressors	$770 (power, kW)$^{0.96}$ + $400 (power, kW)$^{0.6}$ assume 70% efficiency
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	$[1.67(0.959 + 0.041$P$ - 8.3×10^{-6}P^2)]×10^z $z = (3.17 + 0.2D + 0.5 \log_{10}L + 0.21 \log_{10}L^2)$ D = diameter, m 0.3 m < D < 4.0 m L = height, m 3 < L/D < 20 P = absolute pressure, bar
Reactor	assume to be $1 million
Tanks	1000V$^{0.6}$ V = volume, m^3

Equipment Cost Factors

Pressure Factors

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

Material Factors

Carbon Steel	0.0
Stainless Steel	4.0

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

Heat Exchangers

For heat exchangers that do not have to be designed in detail, use the following approximations for heat transfer coefficients to allow you to determine the heat transfer area and heat exchanger cost.

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

Other Information

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

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 written using a word processor. Three identical copies should be submitted, one for each instructor. The written project reports are due by 11:00 a.m. Thursday, November 29, 2001. Late projects will receive a minimum of a one letter grade deduction.

The report should be clear and concise. For the correct formatting information, refer to the document entitled *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 "mini-design." These may be hand written if done neatly. Calculations that cannot be easily followed will lose credit.

Since this project involves "mini-designs," it is suggested that the report be organized as follows. There should be a general abstract and introduction. Then, there should be a results section followed by a discussion section for each "mini-design." General conclusion and recommendation sections should follow. At a minimum, there should be an appendix for each of the "mini-designs." With this organization, there is no need for a separate section of the report for each class, as suggested in the document entitled *Written Design Reports*.

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. Each group member should speak only once. A 5-10 minute question-and-answer session will follow, and all members must participate. Refer to the document entitled *Oral Reports* for instructions. The oral presentations will be November 29, 2001, from 11:00 a.m. to 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 310, ChE 311, and ChE 320***.

Anyone not participating in this project will automatically receive an F for ChE 310, ChE 311, and ChE 320, regardless of other grades earned in these classes.

Groups

You will do this project in a group of three or four. You have already selected a partner, and groups of two have been paired up by the instructors. Since there are 27 students doing the project, there will be 7 groups. There will be 6 groups of 4 and 1 group of 3.

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.