Numerical Methods, Energy Balances

Design Project

Production of Dimethyl Ether

Process Description

Figure 1 is a preliminary process flow diagram (PFD) for the dimethyl ether production process. The raw material is methanol, which may be assumed to be pure. The feed plus recycle is pumped in P-201; heated, vaporized, and superheated in a heat exchanger (E-201); and then sent to the reactor (R-201) in which dimethyl ether (DME) is formed. The reaction that occurs is shown below. The reactor effluent is cooled and partially condensed in a heat exchanger (E-202), and it is then sent to the separation section. In T-201, "pure" DME is produced in the top stream (distillate), with methanol and water in the bottom stream (bottoms). In T-202, the distillate contains methanol for recycle, and the bottoms contains waste water. The desired dimethyl ether production rate is 100,000 tonne/y.

Process Details

Feed Stream

Stream 1: methanol, from storage tank at 1 atm and 25°C, may be assumed pure

Effluent Streams

Stream 7: dimethyl ether product, required 100,000 tonne/y, may be assumed pure

Stream 10: waste water stream, may be assumed pure in material balance calculations, is not pure, so there is a cost for its treatment

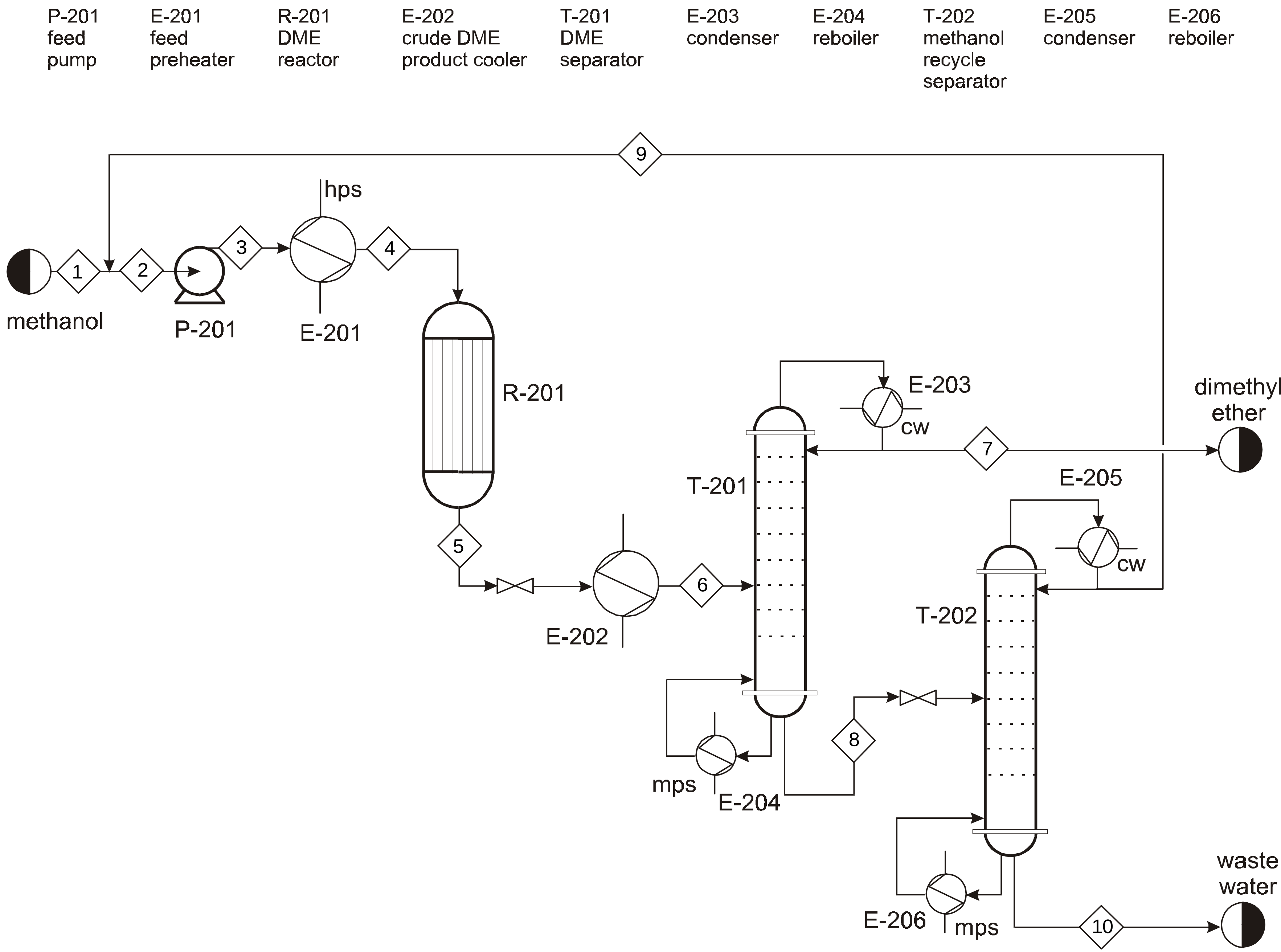
Equipment

Pump (P-201)

The pump increases the pressure of the feed plus recycle to a minimum of 15 bar.

Heat Exchanger (E-201):

This unit heats, vaporizes, and superheats the feed to 250°C at 15 bar. The source of energy for heating must be above 250°C.



Unit 200 - Dimethyl Ether Process

Reactor (R-201):

The following reaction occurs:

$$\underset{\text{methanol}}{2CH_3COOH} \underset{\leftarrow}{\longrightarrow} \underset{\text{dimethyl ether}}{CH_3OCH_3} + H_2O \qquad (1)$$

The reaction is equilibrium limited. The conversion is 80% of the equilibrium conversion at the pressure and exit temperature of the reactor. Based on the catalyst and reaction kinetics, the reactor must operate at a minimum of 15 bar. The reactor operates adiabatically, and, since the reaction is exothermic, the reactor effluent temperature will be above 250°C. If you choose, you may run the reactor isothermally, in which case you need a medium to remove the heat generated, and that medium must always be at a lower temperature than that of the reactor.

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

$$\ln K = -2.205 + \frac{2708.6317}{T} \qquad (2)$$

where the temperature is in Kelvin.

Heat Exchanger (E-202):

This unit cools and partially condenses the reactor effluent. The valve before this heat exchanger reduces the pressure. This exit pressure may be at any pressure below the reactor pressure, but must be identical to the pressure at which T-201 operates.

Distillation Column (T-201):

This distillation column separates DME from methanol and water. For this semester only, the separation may be assumed to be perfect, i.e., pure DME is produced in the distillate. The temperature of the distillate is the temperature at which DME condenses at the chosen column pressure. For this project only, you may use the Antoine's Equation constants for DME given in Felder and Rousseau[1] up to 50°C.

Heat Exchanger (E-203):

In this heat exchanger, the contents of the top of T-201 (pure dimethyl ether) are condensed from saturated vapor to saturated liquid at the column pressure at a rate three times the flow of Stream 7. One-third of the condensate becomes Stream 7 and the remainder is returned to the column. The cost is 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-204):

In this heat exchanger, you may assume that one-half of the flow of Stream 8 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 bubble point temperature of the methanol-water mixture at the column pressure. The cost is for the amount of steam needed to supply the necessary heat. The steam temperature must be above the temperature of the vaporizing stream.

Distillation Column (T-202):

This distillation column separates methanol for recycle from water. For this semester only, the separation may be assumed to be perfect. However, since we know this cannot be true in practice, the water stream is actually a waste water stream, and there is a cost for its treatment. The temperature of the distillate is the temperature at which methanol condenses at the chosen column pressure. The valve before T-202 is optional. It is needed if the pressure of T-202 is chosen to be lower than that of T-201. If the pressures are the same, the valve can be eliminated. If you desire a higher pressure in T-202, you must add a pump in place of the valve.

Heat Exchanger (E-205):

In this heat exchanger, the contents of the top of T-202 (pure methanol) are condensed from saturated vapor to saturated liquid at the column pressure at a rate three times the flow of Stream 9. One-third of the condensate becomes Stream 9 and the remainder is returned to the column. The cost is 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-206):

In this heat exchanger, you may assume that one-half of the flow of Stream 10 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. The cost is 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.

Utility Costs

Low-Pressure Steam (446 kPa, saturated)	\$5.00/1000 kg
Medium-Pressure Steam (1135 kPa, saturated)	\$7.31/1000 kg
High-Pressure Steam (4237 kPa, saturated)	\$8.65/1000 kg
Natural Gas or Fuel Gas (446 kPa, 25°C)	\$3.00/GJ
Electricity	\$0.05/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 should be 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
Process Water available at 300 kPa and 25°C	\$0.04/1000 kg
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 DME: 145 J/mol K

Vapor Heat Capacity

for DME: $17.02 + 0.1791T - 5.234 \quad 10^{-5}T^2 - 1.918 \quad 10^{-9}T^3$ J/mole K T (K)

Normal Heat of Vaporization

for DME: $2.6 \quad 10^4$ J/mol

Heat of Formation

for DME: -1.842 10^5 J/mol

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 cost for dimethyl ether is $0.43/lb. The cost for methanol is $0.60/gal.

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 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 38. 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. 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 18, 2001, 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 23, 2001, at 1:00 p.m. The oral reports will be Monday, April 23, 2001 (ChE 38 class) and Wednesday, April 25, 2001 (ChE 41 class). There will be a project review on Friday, April 27, 2001 (ChE 41 class). In addition, everyone must attend the senior design presentation at 2:30 pm on Thursday, April 26, 2001. 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 38 and ChE 41.

Anyone not participating in this project will automatically receive an F for ChE 38 and ChE 41, 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.

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

Equipment	**Installed Cost in thousands of $**
Reactor (per stage)	1000
Distillation Columns, each (without peripheral heat exchangers)	500
Compressors, each	1000
Heat Exchangers, each (included ones associated with distillation columns)	50
Vessels, each	50
Pumps, each	10

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