CHE654 – Plant Design Project #5
Semester 1, 2023

DESIGN OF A DIMETHYL ETHER PRODUCTION PROCESS

(Courtesy of the Department of Chemical Engineering at West Virginia University, USA)

Introduction

Dimethyl ether (DME) is used primarily as a propellant. It is miscible with most organic solvents and has high solubility with water. Recently, the use of DME as a fuel additive for diesel engines has been investigated due to its high volatility (desirable for cold starting) and high cetane number.

DME is produced by the catalytic dehydration of methanol over zeolite catalyst. The reaction is as follows:

$$2CH_3OH = CH_3OCH_3 + H_2O$$

In the temperature range of normal operations, there are no side reactions. A simplified process flow diagram for a DME process is shown in Figure 1. Your job is to analyze the simplified dimethyl ether production process, to suggest profitable operating conditions, and to write a final report summarizing your findings. Note that although you are to look for a "best" solution in your design, optimization is NOT required in this design project.

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; must be 95.5 wt% 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.

Reactor (R-201):

The following reaction occurs:

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

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

$$\ln K = -2.205 + \frac{2708.6317}{T} \tag{2}$$

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. The temperature of the distillate is the temperature at which DME condenses at the chosen column pressure.

Heat Exchanger (E-203):

In this heat exchanger, the contents of the top of T-201 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. Since we know the separation between methanol and water cannot be perfect 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.

Design of Heat Exchangers, E-201 and E-202

A detailed design of E-201 and E-202 is required for base-case conditions. It should be assumed that cooling water and other utilities are available at the conditions specified in the Appendix of this problem statement. For this heat exchanger design, the following information should be provided:

- Diameter of shell
- Number of tube and shell passes
- Number of tubes per pass
- Tube pitch and arrangement (triangular/square/..)
- Number of shell-side baffles, if any, and their arrangement (spacing, pitch, type)
- Diameter, tube-wall thickness, shell-wall thickness, and length of tubes
- Calculation of both shell- and tube-side film heat transfer coefficients
- Calculation of overall heat transfer coefficient (you may assume that there is no fouling on either side of the exchanger)
- Heat transfer area of the exchanger
- Shell-side and tube-side pressure drops (calculated, not estimated)
- Materials of construction
- Approximate cost of the exchanger

A detailed sketch of the two exchangers should be included along with a set of comprehensive calculations in an appendix for the design of the heat exchangers. You should use ASPEN Exchanger Design & Rating (EDR) in the ASPEN Plus simulator to carry out the detailed design.

Economic Analysis

When evaluating alternative cases, you should carry out an economic evaluation and profitability analysis based on a number of economic criteria such as payback period, internal rate of return, and cash flow analysis. In addition, the following objective function should be used. It is the equivalent annual operating cost (EAOC), and is defined as

EAOC = – (product value – feed cost – other operating costs – 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, although you are **not** being asked to carry out optimization.

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. The capital cost annuity is defined as follows:

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

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, $n = 10$.

For detailed sizing, costing, and economic evaluation including profitability analysis, you may use the Aspen Process Economic Analyzer (formerly Aspen Icarus Process Evaluator) in Aspen Plus Version 8. However, it is also a good idea to independently verify the final numbers based on other sources such as cost data given below.

Other Information

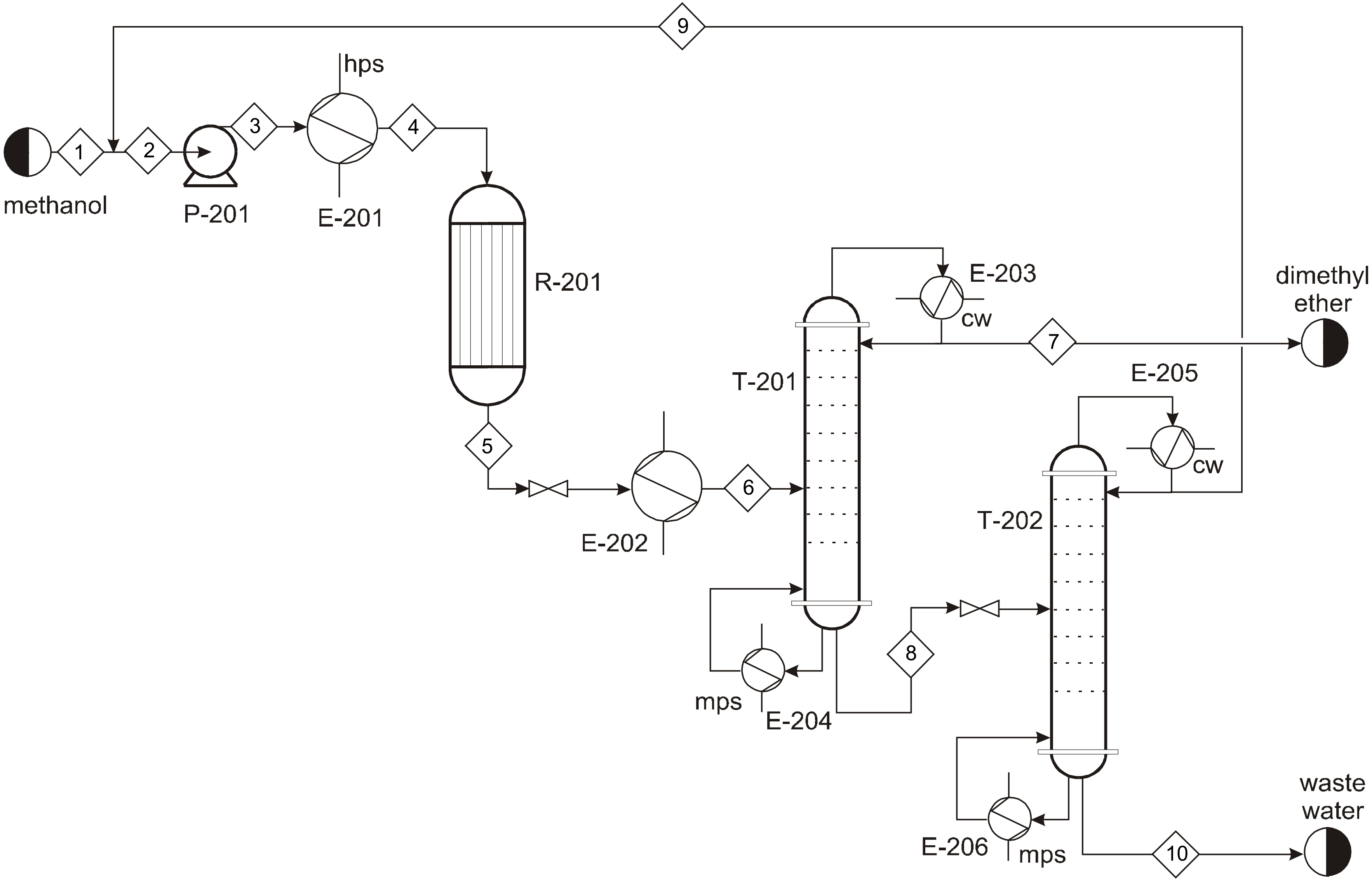
You should assume that a year equals 8,000 hours. This is about 330 days, which allows for periodic shut-down and maintenance.

Final Comments

As with any open-ended problem; i.e., a problem with no single correct answer, the problem statement above is deliberately vague. You may need to fill in some missing data by doing a literature search, Internets search, or making assumptions. 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.

Moreover, in some areas (e.g. sizing/costing) you are given more data and information than what is needed. You must exercise engineering judgment and decide what data to use. Also you should also seek additional data from the literature or Internet to verify some of the data, e.g. the prices of products and raw materials.

P-201	E-201	R-201	E-202	T-201	E-203	E-204	T-202	E-205	E-206
feed pump	feed preheater	DME reactor	crude DME product cooler	DME separator	condenser	reboiler	methanol recycle separator	condenser	reboiler



Unit 200 - Dimethyl Ether Process

Cost 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\times10^5$ (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

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

mixed alcohol feed	\$0.70/gal
pure alcohols	see *Chemical Market Reporter*

Products

dimethyl ether	\$1.00/kg
diethyl 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 Credit use this price for fuel gas credit	\$2.50/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	\$20/GJ
Deionized Water available at 5 bar and 30°C	\$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit
Refrigeration	\$60/GJ
Wastewater Treatment	\$50/1000 m^3

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

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

References

1. Felder, R. M. and R. W. Rousseau, *Elementary Principles of Chemical Processes*, 2nd edition, Wiley, New York, 1986.

2. Perry, R. H. and D. Green, eds., *Perry's Chemical Engineers' Handbook*, 7th edition, McGraw-Hill, New York, 1997.

3. Butt, J. B., H. Bliss, and C. A. Walker, "Rates of Reaction in a Recycling System – Dehydration of Ethanol and Diethyl Ether Over Alumina," *AIChE-J*, **8**, 42-47 (1962).

4. Berčič, G. and J. Lavec, "Intrinsic and Global Reaction Rates of Methanol Dehydration over γ-Al_2O_3 Pellets," *Ind. Eng. Chem. Res*., **31**, 1035-1040 (1992).