Fluid Mechanics, Heat Transfer, Fluid Mechanics
Design Project

Production of Ethanol

Your assignment is to continue evaluating the details of a process to produce 30,000 tonne/y of ethanol from ethylene. This is the amount of ethanol in the product stream, not the total mass of the product stream.

A suggested process flow diagram (PFD) is shown in Figure 1. You should use this as a starting point. Your assignment is to complete the mini-designs described later in this document.

Chemical Reaction

Unit 200 produces ethanol from ethylene using a catalytic reaction. Figure 1 illustrates the current process.

The reaction that occurs in the reactor is reversible

$$C_2H_4 + H_2O \leftrightarrow C_2H_5OH \qquad (1)$$

Ethylene is available from a pipeline at 5000 kPa and 25°C. It is mixed with a hot recycle stream and subsequently mixed with boiler feed water (extremely pure) that has already been pumped to 5000 kPa at 90°C. The reactor feed is heated, reacted adiabatically, and cooled. The cooled reactor effluent is passed through a throttling valve to reduce the pressure to 500 kPa. In V-201, light gases are separated into Stream 9, and the ethanol/water mixture produced in Stream 10 is sent for further purification. Some of Stream 9 is recycled and some is purged.

Process Details

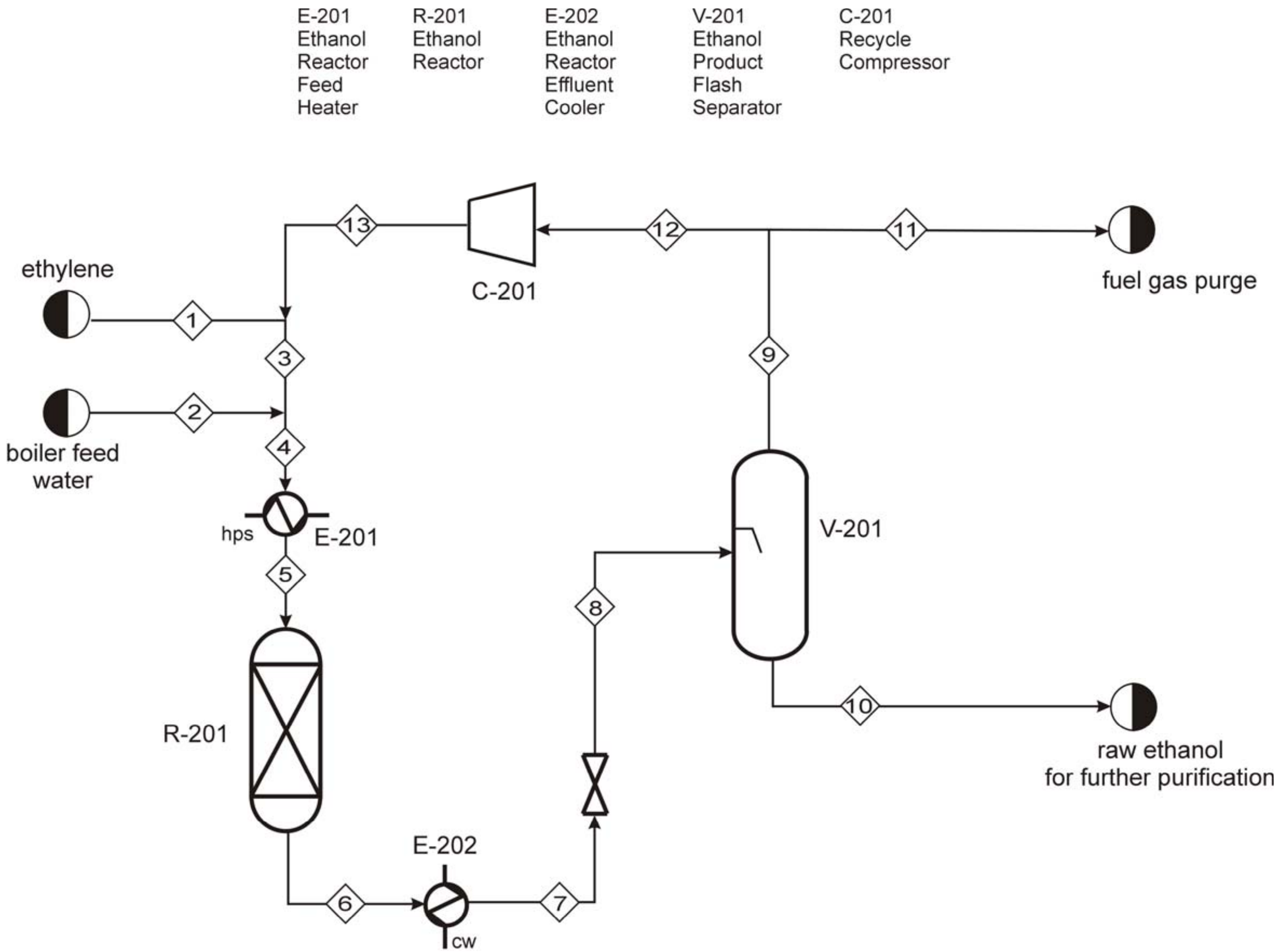
Feed Stream and Effluent Streams

Stream 1: Ethylene – at 25°C and ≤5000 kPa – contains 1 wt % ethane impurity

Stream 2: Boiler Feed Water – at 90°C and ≤5000 kPa – very pure water

Stream 10: ethanol in water for further purification – 30,000 tonne/y of ethanol in this stream

Stream 11: purge fuel-gas to furnace – may take credit for lower heating value – for the base case, use 90% recycle to 10% purge



Unit 200 Ethanol Production Process

Equipment Information

Heat Exchanger (E-201)

The reactor feed is heated to 200°C using high-pressure steam.

Reactor (R-201)

This is an adiabatic, packed bed reactor. For this project, 20% conversion is assumed. The base-case inlet pressure is 5000 kPa minus the pressure losses in the pipes, and the reactor pressure drop is 50 kPa.

Heat Exchanger (E-202)

This heat exchanger cools and partially condenses the reactor effluent. The base-case temperature is 50°C. The subsequent valve reduces the pressure to 500 kPa in the base case. The temperature and pressure may be optimized.

Vessel (V-201)

This vessel separates the light gases from ethanol and water at the conditions of Stream 8. The vapor exits in the top stream, and the liquid exits in the bottom stream. Assume a 10-minute liquid residence time for sizing considerations. This means that the flowrate of the liquid stream exiting in Stream 10 is used to calculate a volume. Then, this volume is doubled to allow space for the vapor to disengage from the liquid.

Compressor (C-201)

The compressor increases the pressure of the recycle stream to the pressure of the feed streams, and it has an efficiency of 70%.

Assignment

The assignment consists of the following "mini-designs."

1. Fluid Mechanics and Heat Transfer

<u>Design Problem</u>

You are to optimize the design of the feed section of the process, which includes Streams 1, 2, 3, 4, 5, and 13 along with E-201. The stream conditions should be taken from the base-case simulation performed in Section 4. For exchanger E-201, a detailed design is required. For the optimization portion, heat transfer areas (and subsequently costs) may be estimated using the following overall heat transfer coefficients:

Liquid-liquid = 250 $W/m^2°C$

Boiling liquid-liquid = 600 W/m^2°C
Gas-liquid = 60 W/m^2°C
Condensing gas-liquid = 500 W/m^2°C

For the final, detailed design of the heat exchanger (E-201), heat transfer coefficients must be calculated.

The objective function for the optimization should be the Equivalent Annual Operating Cost (*EAOC*, $/y) for this section only, that is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC \tag{2}$$

where *CAP* ($) is the capital investment for all the equipment (includes pumps, compressors, heat exchanger, piping, valves, etc.), *AOC* ($/y) is the annual operating cost (includes utility costs for heat exchanger, compressor, and pump), and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{3}$$

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

The costs for the piping components and heat exchanger are given in the Appendix. The optimal pipe diameter and schedule number of each stream, the heat exchanger area, and the heat exchanger tube size/pitch that minimizes the EAOC must be determined. For streams with no phase change, the pressure drops for each exchanger may be estimated from:

15 kPa for the shell-side fluid if 1 inch 16 BWG tubes at 1.25 in square pitch
35 kPa for the tube-side fluid if 1 inch 16 BWG tubes

For other configurations, the pressure drops can be obtained by the scaling methods illustrated in CHE 310 class.

For E-201, will be designed in detail, the approximate pressure drops may be used in the calculations to determine optimal pipe diameter. However, in the detailed heat exchanger design, the pressure drops must be calculated using the appropriate relationships.

In order to evaluate the amount of piping required for the mini-design, it may be assumed that E-201 is 2 m above grade (ground level), that a compressor is located at grade with the inlet 0.3 m above grade and the outlet 1 m above grade, and that a pump is located at grade with the inlet 0.2 m above grade and the outlet 0.5 m above grade. E-201 is located 3 m of equivalent length from the mixing point for Streams 2 and 4 with the mixing point 2 m above grade. The contract with our ethylene supplier requires that the pressure at our plant boundary be 8000 kPa, and the plant boundary is 75 m of equivalent length from the mixing point with Stream 13. The specified pressure of boiler feed water is at a point 25 m of equivalent length from the mixing point with Stream 3. The equivalent length of the pipe for Stream 13 is 8 m, the pipe for Stream 3 is a straight run of 1 m, and the equivalent length of the pipe for Stream 5 is 12 m.

Design of Heat Exchanger, E-201

A detailed design of E-201 is required, which may be done for base-case conditions. It should be assumed that 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, 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 exchanger should be included along with a set of comprehensive calculations in an appendix to the mini-design.

2. Thermodynamics – (ChE 320)

You are to optimize the flash and recycle system, which includes Streams 8, 9, 11, 12, and 13 along with C-201 and V-201. The objective function for the optimization should be the Equivalent Annual Operating Cost (*EAOC*, \$/y) for this section only, that is defined as:

$$EAOC = CAP\left(\frac{A}{P}, i, n\right) + AOC \tag{2}$$

where *CAP* (\$) is the capital investment for the equipment (includes compressors, heat exchangers, vessel, etc.), *AOC* (\$/y) is the annual operating cost (includes utility costs for compressor as well as the reactant feed cost), and

$$\left(\frac{A}{P}, i, n\right) = \frac{i(1+i)^n}{\left[(1+i)^n - 1\right]} \tag{3}$$

where i = 0.15 (15% rate of return) and n = 10 (ten-year plant life). Optimization variables can include, but are not limited to the vessel pressure and temperature, and the recycle-to-purge ratio. The equipment costs and efficiencies are found in the Appendix and current contract prices for ethylene can be found in the "Key Indicators" section of *ICIS Chemical Business*. *ICIS* provides a list of indicative prices for student use at (http://www.icis.com/StaticPages/a-e.htm), but these prices are only to be used as a rough guide. The recent price fluctuations in the oil market have led to similar price fluctuations in ethylene since it is a product of refining. Please use the contract bulk price as published in the September 29 print issue for *EAOC* calculations. The Evansdale Library maintains a subscription.

Additionally, we must be able to model accurately the thermodynamics of the water-ethanol-ethylene mixture that enters the flash vessel. Inaccuracies in the thermodynamics of the vapor-liquid equilibrium of this mixture can lead to inaccurate calculations of the phase separation and the overall cost of the plant. Justify your choice of thermodynamics package based on an examination of the *T-xy* diagrams of the pairs of components at a variety of possible operating pressures.

3. Safety Analysis Report

When designing a chemical process, it is important to know the properties of the chemicals being consumed and produced in the process. The reactivity and toxicity of the reactants and products will not only affect the design but will also affect the procedures that might be implemented during an unscheduled event such as an emergency shutdown. The purpose of the safety analysis report is to make management aware of risks to personnel due to the flammability and toxicity of all chemicals consumed or produced in the process. As a minimum, the MSDS (material and safety data sheets) for all these chemicals should be provided in an appendix, and a brief discussion of the major concerns for each chemical should be given as a separate section of the report. This should include general concerns and concerns that are specific to the operating conditions in this process. In addition, a brief discussion of possible safety hazards for each piece of equipment in your process should be provided. Finally, a feature of your process design that addresses one of these concerns should be explained.

4. Chemcad/Process Improvements

A Chemcad simulation of the base case of the process shown in Figure 1 should be provided. Process improvements that do not violate the laws of physics may be suggested. An explanation of the rationale for such process improvements should be provided, including an economic analysis, if possible.

Other Information

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

Suggested Plan of Attack

The safety analysis can begin as soon as the project is distributed. A good place to find MSDS sheets is http://siri.org. The Chemcad simulation can also be done immediately.. The fluid mechanics/heat transfer design and the thermodynamics design can be started next. The vapor-liquid equilibrium analysis should not be attempted until that material is covered in thermodynamics class.

Deliverables

Written Reports

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 20, 2008. 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*. The report must contain a labeled process flow diagram (PFD) and a stream table, each in the appropriate format. The preferred software for preparing PFDs is Corel Draw. A PFD from Chemcad is unacceptable; however, it should be included in the appendix along with a Chemcad report for the base case. Figure 1 should be used as a template for your PFD. 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-project." These may be hand written if done neatly. Alternatively, Excel spreadsheets may be included, but these must be well documented so that the reader can interpret the results. Calculations that cannot be easily followed and that are not explained 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 one appendix for each of the "mini-designs" with detailed calculations that are clearly written and easy to follow.

In order to evaluate each group member's writing skills, the results and discussion sections for each mini-design should be written by a different group member. The authorship of each of these mini-reports should be clearly specified in the report. Although the individual written portions of the reports must be authored by a single group member, it is the intent of the instructors that group members should help each other in writing different sections. To this end, we recommend that you seek input, such as proofreading and critiques, from other members of your group.

The reports will be evaluated as follows:

- course-specific technical content – 50%

- oral presentation – 20%
- written report – 20%
- technical quality of general sections (safety, simulation, etc.) – 10%

For a more detailed set of evaluation criteria that we will use, see the following web site (design project assessment, oral report assessment, written report assessment):
http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php

Each report will be assessed separately by each of the three instructors. A historical account of what each group did is neither required nor wanted. Results and explanations should be those needed to justify your choices, not a litany of everything that was tried. Each mini-report should be limited to 4-5 double space pages plus figures and tables.

Oral 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 Friday November 21, 2008, from 11:00 a.m. to 1:00 pm. 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***.

Teams

This project will be completed in teams of 3 or 4. More details of group formation and peer evaluation will be discussed in class.

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 the project proceeds, questions from the class will require revisions and/or clarifications. It is important to be aware that these revisions/clarifications may be forthcoming.

Appendix
Economic Data

Equipment Costs (Purchased)

Note: The numbers following the attribute are the minimum and maximum values for that attribute. For a piece of equipment with a lower attribute value than the minimum, the minimum attribute value should be used to compute the cost. For a piece of equipment with a larger attribute value, extrapolation is possible, but inaccurate. To err on the side of caution, the price for multiple, identical, smaller pieces of equipment should be used.

Pumps $\log_{10}(\text{purchased cost}) = 3.4 + 0.05\log_{10} W + 0.15[\log_{10} W]^2$
W = power (kW, 1, 300)
assume 80% efficiency

Heat Exchangers $\log_{10}(\text{purchased cost}) = 4.6 - 0.8\log_{10} A + 0.3[\log_{10} A]^2$
A = heat exchange area (m^2, 20, 1000)

Compressors $\log_{10}(\text{purchased cost}) = 2.3 + 1.4\log_{10} W - 0.1[\log_{10} W]^2$
W = power (kW, 450, no limit)
assume 70% efficiency

Compressor Drive $\log_{10}(\text{purchased cost}) = 2.5 + 1.4\log_{10} W - 0.18[\log_{10} W]^2$
W = power (kW, 75, 2600)

Turbine $\log_{10}(\text{purchased cost}) = 2.5 + 1.45\log_{10} W - 0.17[\log_{10} W]^2$
W = power (kW, 100, 4000)
assume 65% efficiency

Fired Heater $\log_{10}(\text{purchased cost}) = 3.0 + 0.66\log_{10} Q + 0.02[\log_{10} Q]^2$
Q = duty (kW, 3000, 100,000)
assume 80% thermal efficiency
assume can be designed to use any organic compound as a fuel

Vertical Vessel $\log_{10}(\text{purchased cost}) = 3.5 + 0.45\log_{10} V + 0.11[\log_{10} V]^2$
V = volume of vessel (m^3, 0.3, 520)

Horizontal Vessel $\log_{10}(\text{purchased cost}) = 3.5 + 0.38\log_{10} V + 0.09[\log_{10} V]^2$
V = volume of vessel (m^3, 0.1, 628)

Storage Tanks $\log_{10}(\text{purchased cost}) = 4.85 - 0.397\log_{10} V + 0.145[\log_{10} V]^2$
V = volume of tank (m^3, 90, 30000)

Additional Cost Information

Piping straight pipe $/m = 5.0 (nominal pipe diameter, in)$(1+(\text{sch }\#)/20)^{0.25}$
sch = schedule number for pipe
use the same sch number for fittings and valves

fittings (except valves) $/fitting = 50.0 (nominal pipe diameter, in)$(1+(\text{sch }\#)/20)^{0.25}$

Valves for gate (isolation) valves $100 (nominal pipe diameter, in)$^{0.8}$ $(1+(\text{sch }\#)/20)^{0.25}$
for control valve use $1000 (nominal pipe diameter, in)$^{0.8}$$(1+(\text{sch }\#)/20)^{0.25}$

Utility Costs

Low-Pressure Steam (618 kPa saturated)	$13.28/GJ
Medium-Pressure Steam (1135 kPa saturated)	$14.19/GJ
High-Pressure Steam (4237 kPa saturated)	$17.70/GJ
Natural Gas (446 kPa, 25°C)	$11.00/GJ
Fuel Gas Credit	$9.00/GJ
Electricity	$0.06/kWh
Boiler Feed Water (at 549 kPa, 90°C)	$2.45/1000 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	$0.354/GJ
Refrigerated Water available at 516 kPa and 10°C return pressure ≥ 308 kPa return temperature is no higher than 20°C	$4.43/GJ
Deionized Water available at 5 bar and 30°C	$1.00/1000 kg
Waste Treatment of Off-Gas	incinerated - take fuel credit
Refrigeration	$7.89/GJ
Wastewater Treatment	$56/1000 m^3

Equipment Cost Factors

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

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

Carbon Steel	MF = 0.0
Stainless Steel	MF = 4.0