Energy Balances and Numerical Methods
Design Project

Ethanol Production

Your assignment is to continue to evaluate the feasibility of a process to produce 30,000 tonne/y of ethanol from ethylene.

A suggested process flow diagram (PFD) is shown in Figure 1. You should use this as a starting point. Your assignment is to develop a “best” case, where “best” is dependent upon economic considerations, *i.e*., EAOC. In reporting your best case, clearly indicate any modifications to the PFD and state the operating conditions for the modified process and the corresponding EAOC.

Chemical Reaction

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

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, all of the ethylene and ethane and some of the ethanol and water enters Stream 9. Some of Stream 9 is recycled and some is purged. Stream 10 is distilled further to produce 90 mol % “crude” ethanol and a waste water stream that must be sent to waste treatment.

The reaction that occurs in the reactor is reversible

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

This is an equilibrium reaction, and the equilibrium conversion (X_{eq}) of ethylene is obtained by solving

$$(KP+1)X_{eq}^2 - [(KP+1)(N+1)]X_{eq} + KPN = 0 \qquad (2)$$

where P is the pressure in atm, N is the moles of water/moles ethylene in the reactor feed, and

$$K = 1.27825\times 10^{-7} \exp\left(\frac{47215(\text{kJ/kmol})}{\text{RT(K)}}\right) \qquad (3)$$

In the reactor, 90% of the equilibrium conversion is obtained.

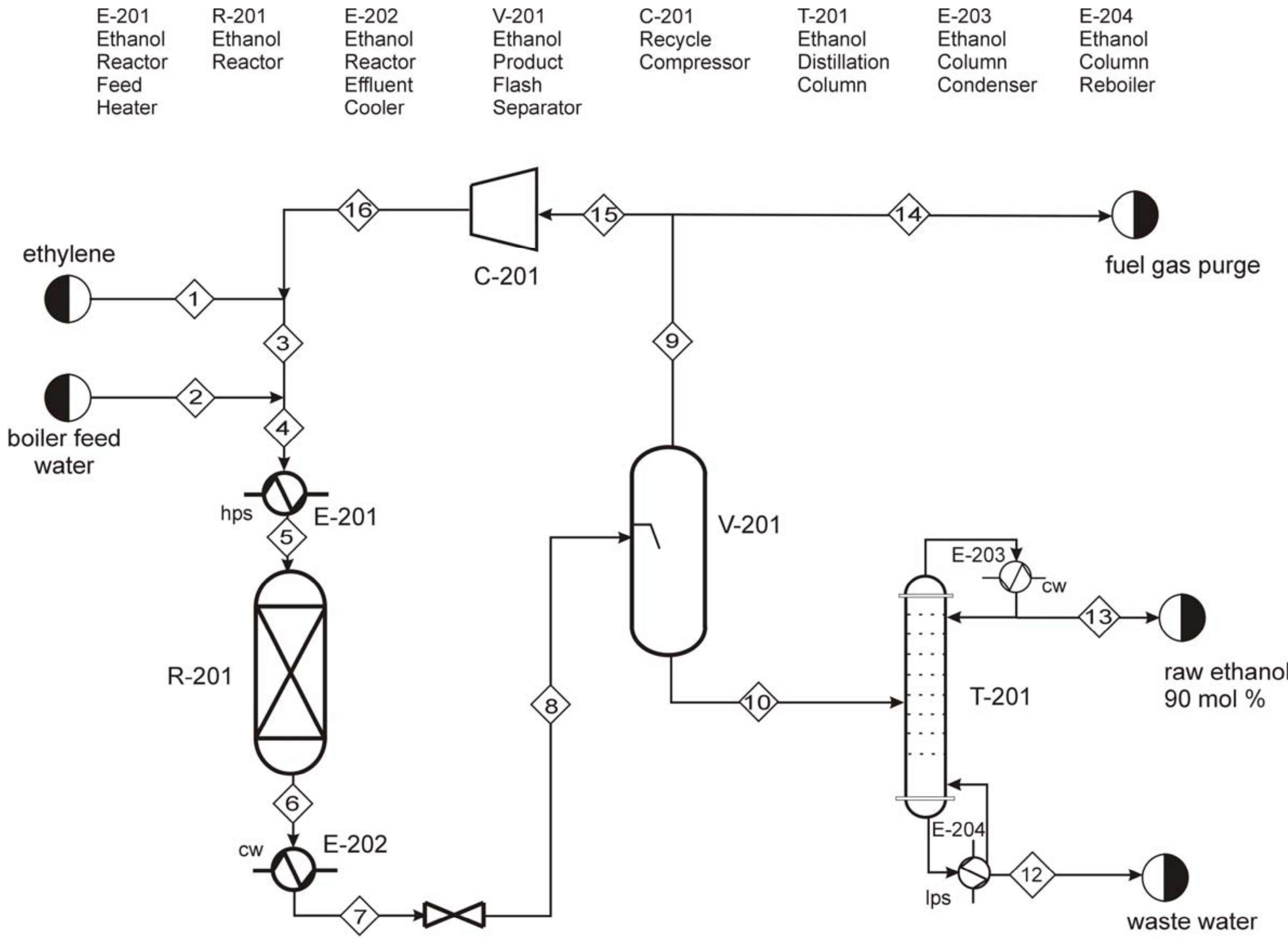

Figure 1: Unit 200 Ethanol Production Process

Process Details

Streams and Equipment Details

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 12: waste water stream – there is a cost for treatment
organic concentration ≤5000 ppm

Stream 13: 90 mol % ethanol in water – 30,000 tonne/y of ethanol in this stream

Stream 14: purge fuel-gas to furnace – may take credit for lower heating value

Equipment Information

Heat Exchanger (E-201)

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

Reactor (R-201)

This is an adiabatic reactor. It is essentially a large pipe packed with catalyst. The equilibrium conversion can be calculated based on a choice of the operating pressure and the outlet temperature. These are decision variables that you are expected to manipulate to find optimum values. The reactor may operate at any pressure ≤8000 kPa and at any temperature above 200°C such that there is no liquid present. The actual conversion in the reactor is 90% of the equilibrium conversion. You will find the conversions to be low, requiring a large recycle stream. An alternative reactor configuration is to stage several adiabatic reactors with a heat exchanger between the stages to reduce the inlet temperature to each subsequent reactor. The number of reactor stages is determined by the economics.

Heat Exchanger (E-202)

This heat exchanger cools and partially condenses the reactor effluent to 50°C. The subsequent valve reduces the pressure to 500 kPa.

Compressor (C-201)

The compressor increases the pressure of the recycle stream to the pressure of the feed streams. The compressor may be assumed to be adiabatic. In that case, the compressor power $\dot{W}_s$ (kW) may be calculated as

$$\dot{W}_s\,(\mathrm{kW}) = 12{,}500\,\dot{m}(\mathrm{kmol/s})\left[\left(\frac{P_{out}}{P_{in}}\right)^{0.286} - 1\right] \tag{4}$$

where $\dot{m}$ (kmol/s) is the total molar flowrate of Stream 15. The cost of electricity to run the compressor is a utility cost. The compressor increases the temperature of the stream being compressed according to

$$\frac{T_{out}}{T_{in}} = \left(\frac{P_{out}}{P_{in}}\right)^{0.286} \tag{5}$$

where T is absolute temperature.

Vessel (V-201)

This vessel allows the vapor and liquid produced in E-202 to be separated. The vapor exits in the top stream, and the liquid exits in the bottom stream. Stream 9 contains all of the ethylene and ethane in Stream 8 plus some water and ethanol. Stream 10 contains 93.3% of the ethanol and 99% of the water in Stream 8.

Distillation Column (T-201)

This column runs at 500 kPa. Separation of ethanol from water occurs in this column. Of the ethanol in Stream 10, 98% is recovered in Stream 13. The composition of Stream 13 is 90 mol% ethanol.

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. For this calculation, 90 mol% ethanol in water is condensed from its dew point temperature to its bubble point temperature at the column pressure. There is a cost for the amount of cooling water needed; this is a utility cost. The cooling water leaving E-203 must always be at a lower temperature than that of the stream being condensed, preferably at least 10°C lower. The ratio of Stream 13 to the stream recycled back to T-202 is 1/12.

Heat Exchanger (E-204)

In this heat exchanger, the some of the contents of the stream leaving the bottom of T-201 and entering E-204 are vaporized and returned to the column. The amount vaporized and returned to the column is equal to the amount in Stream 12. The temperature of these streams is the boiling point of the water at the column pressure. The heat required may be estimated by the heat of vaporization of water column pressure. There is a cost for the amount of steam needed to provide energy to vaporize the stream; this is a utility cost. The steam temperature must always be higher than the temperature of the stream being vaporized, preferably at least 10°C higher.

Economic Analysis

When evaluating alternative cases, the objective function to be used is the Equivalent Annual Operating Cost (EAOC), defined as

EAOC = -(product value - feed cost – utility costs – waste treatment cost - capital cost annuity)

A negative value of EAOC means there is a profit. It is desirable to minimize EAOC; *i.e.*, a large negative value of EAOC is very desirable.

Utility costs are those for steam, cooling water, boiler-feed water, electricity, and waste treatment.

The capital cost annuity is an ***annual*** cost (like a car payment) associated with the ***one-time***, fixed capital cost of plant construction and installation. A list of fixed capital costs on an installed basis ("installed cost") for all pieces of equipment will be provided by mid-March.

The capital cost annuity is defined as follows:

$$capital\ cost\ annuity = FCI\,\frac{i(1+i)^n}{(1+i)^n - 1} \qquad (6)$$

where *FCI* is the installed cost of all equipment; i is the interest rate; and n is the plant life, in [y]. For accounting purposes, take $i = 0.15$ and $n = 10$.

Optimization

You will learn optimization methods in ChE 230. The objective function (EAOC) is defined above. You should consider both topological and parametric optimization.

Topological optimization involves considering different process configurations (such location of process equipment, whether or not to add or remove equipment). You may alter the process configuration in any way that improves the economic performance as long as it does not violate the laws of nature. Determining the optimum number of staged reactors with intercooling is an example of a topological optimization.

Parametric optimization involves determining the best operating parameters for the chosen process topology. It is your responsibility to define appropriate decision variables. It is suggested that you look carefully at the efficient use of raw materials and the purge/recycle ratio for Stream 9 as well as the reactor temperature and pressure. If there are too many decision variables to do a reasonable parametric optimization, it is your responsibility to determine, with appropriate justification, which ones most significantly affect the objective function. Then you should focus on only those decision variables. This is called a Pareto analysis.

Data

All of the required data may be found in the appendix of your textbook [1]. For this project, ***and for this project only***, you may use data that are outside the range of applicability, if necessary. It is suggested that you clearly state this assumption in your written report.

Equipment Costs

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

Equipment	**Installed Cost in $thousands**
Tower, T-201	500
Reactor, per unit	500
Vessel, V-201	100
Any heat exchanger	100
Any pump	40
Any compressor	$0.0189\left(\dot{W}_s[\text{W}]\right)^{0.8}$

Utility Costs

Low-Pressure Steam (618 kPa, saturated, cost or credit) $7.78/GJ

Medium-Pressure Steam (1135 kPa, saturated, cost or credit) $8.22/GJ

High-Pressure Steam (4237 kPa, saturated, cost or credit) $9.83/GJ

Natural Gas or Fuel Gas (446 kPa, 25°C)
- cost $6.00/GJ
- credit $5.00/GJ

Electricity $0.06/kWh

Boiler Feed Water (at 549 kPa, 90°C) $2.45/1000 kg

(There is a cost for boiler feed water only if the steam produced enters process streams. If, on the other hand, the steam produced is subsequently condensed, it can be made into steam again. In that case, there is no net cost for boiler feed water.)

Cooling Water $0.354/GJ

available at 516 kPa and 30°C, return pressure ≥ 308 kPa return temperature should be no more than 15°C above the inlet temperature

Refrigerated Water $4.43/GJ
available at 516 kPa and 5°C, return pressure ≥ 308 kPa
return temperature should be no higher than 15°C

Low-temperature Refrigerant $7.89/GJ
available at -20°C

Very low-temperature Refrigerant $13.11/GJ
available at -50°C

Process (Deionozed) Water $0.067/1000 kg
available at desired pressure and 30°C

Waste Water Treatment $56/1000 m^3
based on total volume treated

Raw Material Costs/Product Value

Raw Material or Product	price
ethylene	0.77/kg
boiler feed water	0.00245/kg
"crude" ethanol	0.97/kg

Other Information

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

Deliverables

Each group must deliver a word-processed report. It should be clear, concise and adhere to the prescribed format. The format is explained in the written report guidelines, provided in a separate document. When presenting results for different cases, graphs are superior to tables. The body of the report should be short, emphasizing only the results and briefly summarizing computational strategies. The report appendix should contain details of calculations that are easy to follow. Calculations that cannot be followed easily will lose credit.

The project is due April 28, 2008, at the beginning of class. There will be oral presentations of project results on that day. Oral presentations will continue on April 30, 2008, only if we are unable to complete all presentations on April 28, 2008. Oral presentation guidelines will be provided in a separate document.

Anyone not participating in this project will automatically receive an F for both ChE 202 and ChE 230, regardless of other grades earned in these classes.

Grading

The report grade for each class will be based on the technical content pertinent to that class, which includes the response to questions during the oral presentation (60%), the oral presentation (20%), and the written report (20%). The grades for the oral presentation and written report will include the quality of the writing, the quality of the oral presentation, and the adherence to the prescribed format (documents to follow). The grade for the oral presentation will be a composite grade for the entire team. Therefore, group preparation and feedback are recommended. The grade for the technical content is self explanatory.

The documents on the following web site provide an indication of the expected attributes of a written design report and oral presentation.

http://www.che.cemr.wvu.edu/ugrad/outcomes/rubrics/index.php

Groups

You will work on this project in groups 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 you work on this problem, your questions will require revisions and/or clarifications. 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, 2005.