Energy Balances and Numerical Methods
Design Project

Production of Formalin

Your assignment is to continue to evaluate the feasibility of a process to produce 50,000 tonne/y of formalin. Formalin is 37 wt% formaldehyde in water. Formaldehyde and urea are used to make urea-formaldehyde resins that subsequently are used as adhesives and binders for particle board and plywood.

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 the modified process and state the operating conditions for the modified process and the corresponding EAOC.

Chemical Reaction

Unit 800 produces formalin (37 wt% formaldehyde in water) from methanol using a silver catalyst process. Figure 1 illustrates the current process.

Air is compressed and preheated, fresh and recycled methanol are pumped and preheated, and these two streams are mixed to provide reactor feed. The feed mixture should be about 39 mole % methanol in air, which is above the upper flammability limit for methanol. (For methanol, UFL = 36 mole %; LFL = 6 mole %.) The methanol-air mixture is not flammable above the UFL or below the LFL. In the reactor, the following two reactions occur:

$$CH_3OH + \tfrac{1}{2}O_2 \rightarrow HCHO + H_2O \tag{1}$$

$$CH_3OH \rightarrow HCHO + H_2 \tag{2}$$

The reaction is catalyzed, and, since the net reaction is exothermic, heat is removed in the reactor. The reactor effluent enters a partial condenser in which most of the methanol, formaldehyde, and water are condensed with the oxygen, nitrogen, and hydrogen remaining in the gas phase. The vessel, V-801, allows the vapor and liquid phases to disengage, with the vapor leaving the process (to be burned to treat the hydrogen) and with the liquid being separated in T-801 to recycle the methanol.

C-801	P-801 A/B	E-801	E-802	R-801	E-803	V-801	T-801	E-804	E-805
feed air compressor	methanol feed pump	methanol preheater	air preheater	formaldehyde reactor	reactor effluent cooler	flash vessel	formaldehyde tower	tower reboiler	tower condenser

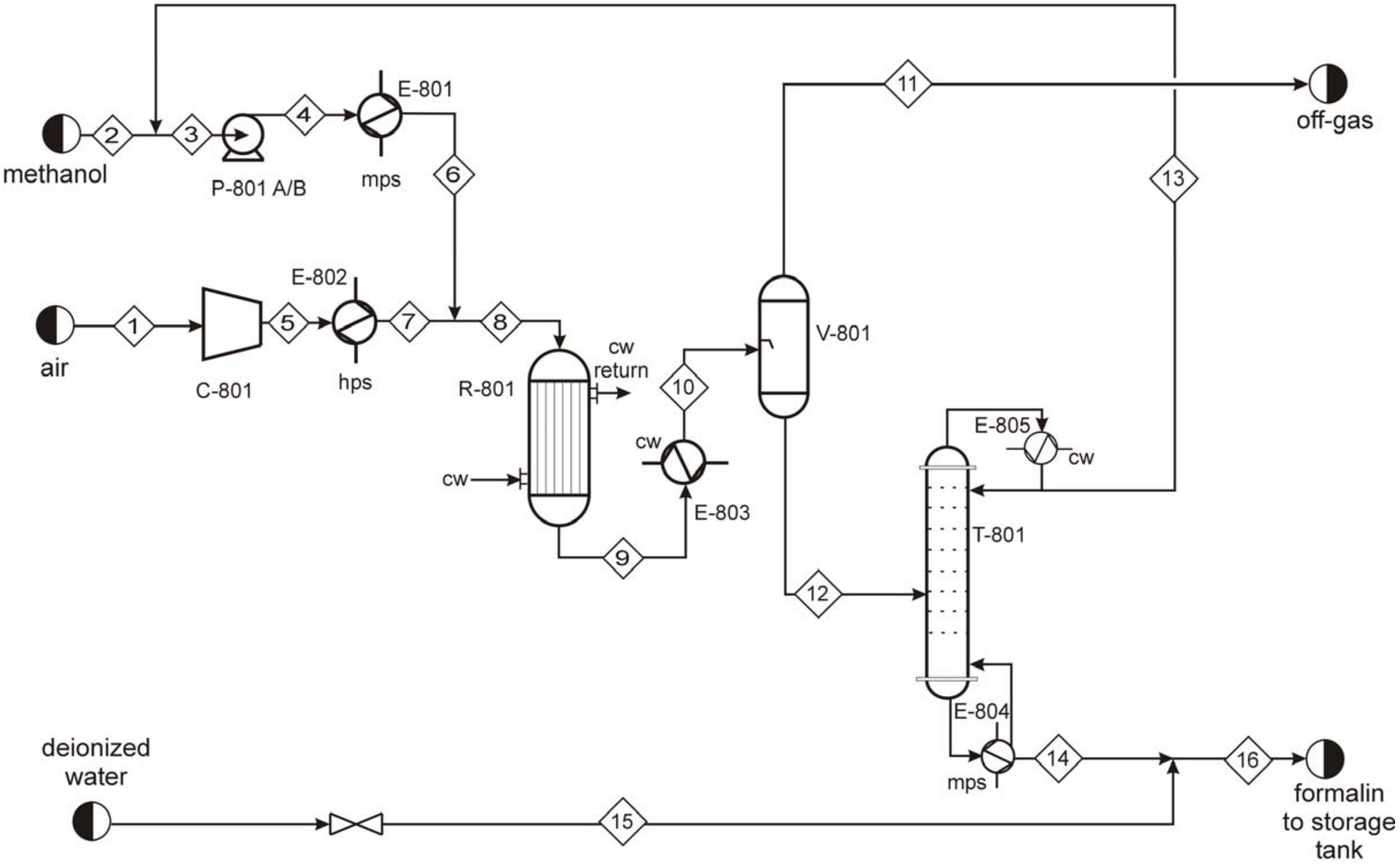

Figure 1: Unit 800 Formalin Production from Methanol

Process Details

Streams and Equipment Details

Stream 1: Air – at 25°C and 1 atm – assumed to contain only O_2 and N_2

Stream 2: Methanol – at 25°C and 1 atm, assumed pure

Stream 8: must be above UFL of methanol, at 200°C, and at a minimum of 200 kPa – Streams 6, 7, and 8 must all be at the same pressure.

Stream 10: The vapor/liquid equilibrium here, which determines how much valuable product and raw material are lost in the off-gas, is a function of pressure and temperature. The pressure is set by the outputs of P-801 A/B and C-801. You are to determine the optimum pressure based on economics, with a minimum pressure of 200 kPa. You are also to determine the optimum temperature of Stream 10 based on economics.

Stream 11: off-gas to furnace

Stream 13: methanol recycle

Stream 14: formaldehyde-water mixture, less than 1 wt% methanol allowed

Stream 15: deionized water

Stream 16: formalin – *i.e.*, 37 wt% formaldehyde in water – This is the stream that must be at a flowrate equivalent to 50,000 tonne/y

Equipment Information

Pump (P-801 A/B)

The pump increases the pressure of Stream 3 to the reactor pressure. The pump work should be calculated using the mechanical energy balance method taught in class. Assume there is no temperature change across the pump. The cost of electricity to run the pump is a utlility cost. The pump efficiency is 80%.

Compressor (C-801)

The compressor increases the pressure of the feed air to the reactor pressure. The compressor may be assumed to be adiabatic. In that case, the compressor work, W_s, may be calculated as

$$W_s = 4.5R(T_{out} - T_{in}) \tag{3}$$

where W_s is in [kJ/kmol] and the inlet and outlet temperatures, T_{in} and T_{out}, respectively, are in [K]. The outlet and inlet temperatures are related through:

$$T_{out} = T_{in}\left(\frac{P_{out}}{P_{in}}\right)^{0.286} \tag{4}$$

The cost of electricity to run the compressor is a utility cost. The compressor efficiency is 70%.

Heat Exchangers (E-801 and E-802)

If needed, these heat exchangers heat the feed streams so that Stream 8 is at the desired reaction temperature.

Reactor (R-801)

Heat must be removed from the reactor so that the outlet temperature is at 200°C. The conversion in the reactor is 100% of the limiting reactant, and the selectivity for the reaction in Equation 1 relative to the reaction in Equation 2 is 9/1.

Heat Exchanger (E-803)

This is a partial condenser, with the primary objective of condensing methanol, formaldehyde, and water. For a given temperature and pressure, you may assume that all light gases enter Stream 11, and that the other components distribute themselves based on a bubble-point calculation.

Vessel (V-801)

This vessel allows the vapor and liquid produced in E-803 to be separated. The vapor exits in the top stream, and the liquid exits in the bottom stream. The Streams 11 and 12 are at the same temperature and pressure as Stream 10. Stream 11 is vapor and Stream 12 is liquid.

Distillation Column (T-801)

This column runs at 1 atm. Separation of methanol from formaldehyde and water occurs in this column. Of the methanol in Stream 12, a sufficient amount enters Stream 13 so that the 1 wt% constraint on Stream 14 is not violated. 99.5% of the formaldehyde and water in Stream 12 enters Stream 14.

Heat Exchanger (E-804)

In this heat exchanger, the some of the contents of the stream leaving the bottom of T-801 entering E-804 are vaporized and returned to the column. The amount returned to the column is equal to the amount in Stream 14. The temperature of these streams is the boiling point of the formaldehyde/water stream at the column pressure. The heat required may be estimated by the heat of vaporization of each component at the boiling point of water at 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.

Heat Exchanger (E-805)

In this heat exchanger, the contents of the top of T-801 are condensed from saturated vapor to saturated liquid at the column pressure. For this calculation, you may assume that the pure methanol is condensed at its boiling point 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-805 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-801 is 1/5.

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, deionized water, boiler-feed water, natural gas, and electricity. If there is excess energy in the process so that steam can be made, the steam produced can be returned to the steam plant for an economic credit equal to the cost of purchasing steam.

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:

$$capital\ cost\ annuity = FCI\frac{i(1+i)^n}{(1+i)^n-1} \tag{2}$$

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). Recall that 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. It is suggested that you look carefully at the efficient use of raw materials and the production of steam for use in the formalin process. It is possible to add additional heat exchangers and separation vessels to Stream 11 to improve the separation of raw materials, if it is justified by the economics.

Parametric optimization involves determining the best operating parameters for the chosen process topology. It is your responsibility to define appropriate decision variables. 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. It is suggested that you look carefully at the conditions in V-801 as decision variables, as discussed earlier in the description of Stream 10.

Data

Much of the required data may be found on the CD that came with your textbook [1]. For this project, ***and for this project only***, you may use data on that CD outside the range of applicability shown in the data base, if necessary. It is suggested that you clearly state this assumption in your written report.

The behavior of formaldehyde/water liquid mixtures is unique. According to the published boiling points, formaldehyde is the most volatile, *i.e.*, it has the lowest boiling point, which means that it should leave the top of the distillation column. However, due to significant molecular interactions between formaldehyde and water (think hydrogen bonding), the formaldehyde follows the water, which has the highest boiling point. Therefore, you should consider formaldehyde/water to be a single component with the properties of water (and total “water” composition equal to the sum of the formaldehyde and water compositions) for the bubble-point and E-804 calculations. Furthermore, in a separation, assume that the formaldehyde/water content of an exit stream is in the same ratio as the formaldehyde/water ratio of the feed stream, with the total amount based on the behavior of water. In a vapor phase, formaldehyde and water should be treated as separate components, and the data on the CD may be used.

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	

Equipment Costs

The equipment costs for the ethylbenzene plant are provided. Each cost is for an individual piece of equipment, including installation.

Equipment	Installed Cost in $thousands
Compressor, C-801	3,000
Tower, T-801	1,000
Reactor, R-801	500
Vessel, V-301	150
Any heat exchanger	150
Any pump	40

Raw Material Costs/Product Value

Raw Material or Product	price
methanol	0.29/lb
formalin	0.40/lb

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 23, 2007, at the beginning of class. There will be oral presentations of project results on that day. Oral presentations will continue on April 25, 2007, only if we are unable to complete all presentations on April 23, 2007. 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 grade for the written report portion will include the quality of the writing, the quality of the presentation, and the adherence to the prescribed format. 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 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. Himmelblau, D. M. and J. B. Riggs, *Basic Principles and Calculations in Chemical Engineering (7th ed.)*, Prentice Hall, Englewood Cliffs, NJ, 2004.