Energy Balances and Numerical Methods
Design Project

Production of Ethylbenzene

Ethylbenzene is the primary raw material used to make styrene. Styrene is polymerized into polystyrene, one of the most important polymers in the chemical industry. The usual practice in the chemical industry is to have ethylbenzene and styrene processes on the same site. Like most ethylbenzene/styrene facilities, there is significant heat integration between the two plants. The ethylbenzene reaction is exothermic, so steam is produced, and the styrene reaction is endothermic, so energy is used in the form of steam.

The purpose of this project is to continue a preliminary analysis to determine the feasibility of constructing a chemical plant to manufacture 80,000 tonne/y of ethylbenzene. The raw materials are benzene and ethylene.

A suggested process flow diagram (PFD) is shown in Figure 1. You should use this as a starting point. Your primary task is to recommend operating conditions for heat exchanger E-301 and flash vessel V-301 that maximize the equivalent annual operating cost, or EAOC (This term is defined later). Process improvements that increase the EAOC are also desired. Any changes that you can justify, which not violate the laws of nature, are allowed. 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. Also, state any recommendations you have for additional process improvements that you were not able to incorporate into the process calculations.

Chemical Reaction

The production of EB takes place via the direct addition reaction between ethylene and benzene:

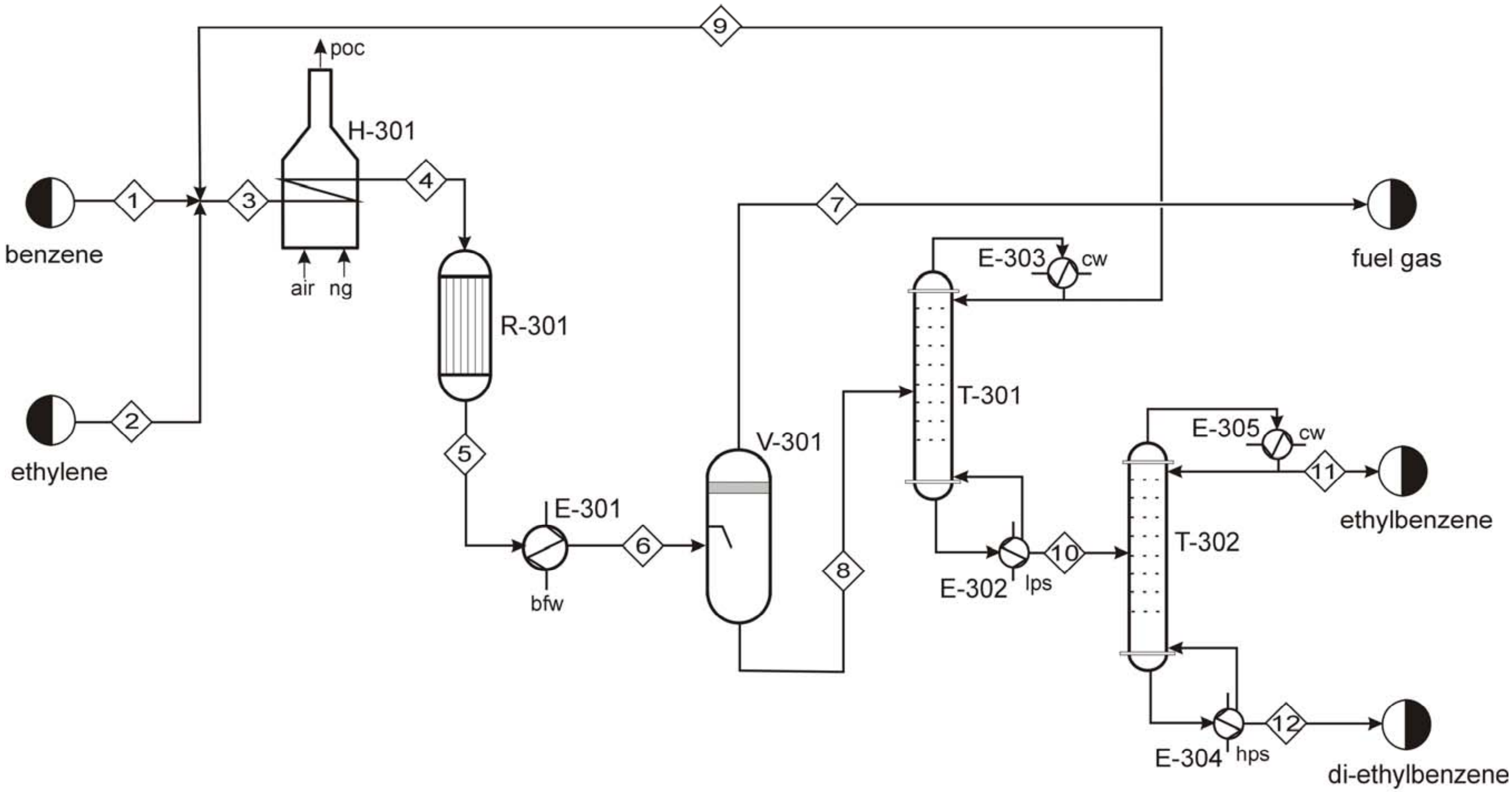
$$\underset{\text{benzene}}{C_6H_6} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{ethyl benzene}}{C_6H_5C_2H_5} \tag{1}$$

The reaction between ethylbenzene and ethylene to produce di-ethylbenzene also takes place:

$$\underset{\text{ethyl benzene}}{C_6H_5C_2H_5} + \underset{\text{ethylene}}{C_2H_4} \rightarrow \underset{\text{diethyl benzene}}{C_6H_4(C_2H_5)_2} \tag{2}$$

Additional reactions between di-ethylbenzene and ethylene yielding tri- and higher ethyl benzene are also possible. However, in order to minimize these additional reactions, the molar ratio of benzene to ethylene is kept high, at approximately 8:1.

H-301 fired heater	R-301 ethylbenzene reactor	E-301 reactor cooler	V-301 flash drum	T-301 benzene tower	E-302 benzene tower reboiler	E-303 benzene tower condenser	T-302 ethylbenzene tower	E-304 ethylbenzene tower reboiler	E-305 ethylbenzene tower condenser



Unit 300: Ethylbenzene Process

Process Details

Streams and Equipment Details

Stream 1: Benzene – at 25°C and 2000 kPa, assumed pure

Stream 2: Ethylene – at 25°C and 2000 kPa, 93 mol % ethylene, 7 mol % ethane

Stream 3: feeds adjusted based on recycle composition to have 8:1 benzene/ethylene ratio

Stream 4: mixed feed heated to 400°C

Stream 5: 100% conversion of limiting reactant in R-301, the selectivity for ethyl benzene production is a function of benzene-to-ethylene ratio. This relationship is expressed as

$$\frac{\xi_2}{\xi_1} = \left(\frac{E_3}{B_3}\right)^{1.2} \tag{3}$$

where ξ_i is the extent of reaction for the reactions in Equations 1 and 2, and the subscript 3 refers to the molar content of ethylene (*E*) and benzene (*B*) of Stream 3. The size of T-301 limits the B_3/E_3 ratio to a maximum value of 12.

Stream 6: vapor/liquid mixture, steam may be produced in E-301, cooling water may also be used, the temperature and pressure of Stream 6 are decision variables

Stream 7: fuel gas purge, credit may be taken for fuel gas based on HHV

Stream 8: mostly benzene, ethylbenzene, and di-ethylbenzene, the sole purpose of V-301 is to allow the vapor and liquid mixture in Stream 6 to separate at the same temperature and pressure as Stream 6

Stream 9: benzene recycle

Stream 10: ethylbenzene/di-ethylbenzene mixture

Stream 11: product ethylbenzene, 2 ppm di-ethylbenzene maximum

Stream 12: di-ethylbenzene to waste treatment

Distillation Column Information

Distillation Column (T-301)

This column runs at 150 kPa. Separation of benzene from ethylbenzene and di-ethylbenzene occurs in this column. Of the benzene in Stream 8, 99% enters Stream 9.

Similarly, 99% of the ethylbenzene and all of the di-ethylbenzene in Stream 8 enters Stream 10.

Heat Exchanger (E-302)

In this heat exchanger, the some of the contents of the stream leaving the bottom of T-301 entering to E-902 are vaporized and returned to the column. The amount returned to the column is equal to the amount in Stream 10. The temperature of these streams is the boiling point of ethylbenzene at the column pressure. The heat required may be estimated by the heat of vaporization of each component at the boiling point of ethylbenzene 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.

Heat Exchanger (E-303)

In this heat exchanger, the contents of the top of T-301 are partially condensed from saturated vapor to saturated liquid at the column pressure. You may assume that benzene and all heavier components condense completely and that any ethylene and ethane present do not condense and are vented from E-903 (not shown) and enter the fuel gas stream. Condensation occurs at the boiling point of each condensing component 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-303 must always be at a lower temperature than that of the stream being condensed. The ratio of Stream 9 to the stream recycled back to T-301 is 1/3.

Distillation Column (T-302)

This column runs at the 150 kPa. Separation of ethylbenzene and di-ethylbenzene occurs in this column. The maximum amount of di-ethylbenzene in Steram 11 is 2 ppm, and 99.9 % of the ethylbenzene in Stream 10 enters Stream 11.

Heat Exchanger (E-304)

In this heat exchanger, the some of the contents of the stream leaving the bottom of T-302 are vaporized and returned to the column. The amount returned to the column is equal to the amount in Stream 12. The temperature of these streams is the boiling point of di-ethylbenzene at the column pressure. The heat required may be estimated by the heat of vaporization of each component at the boiling point of di-ethylbenzene 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.

Heat Exchanger (E-305)

In this heat exchanger, the contents of the top of T-302 are condensed from saturated vapor to saturated liquid at the column pressure. Condensation occurs at the boiling point of each condensing component 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-305 must always be at a lower temperature than that of the stream being condensed. The ratio of Stream 11 to the stream recycled back to T-302 is 2/3.

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, natural gas, and electricity.

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:

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

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 styrene process. It is possible to add additional heat exchangers and separation vessels to Stream 7 to improve the separation of raw materials.

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.

Utility Costs

Low-Pressure Steam (618 kPa, saturated, cost or credit)	\$7.78/1000 kg
Medium-Pressure Steam (1135 kPa, saturated, cost or credit)	\$8.22/1000 kg
High-Pressure Steam (4237 kPa, saturated, cost or credit)	\$9.83/1000 kg
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 available at 516 kPa and 30°C, return pressure ≥ 308 kPa return temperature should be no more than 15°C above the inlet temperature	\$0.354/GJ
Refrigerated Water available at 516 kPa and 5°C, return pressure ≥ 308 kPa return temperature should be no higher than 15°C	\$4.43/GJ
Low-temperature Refrigerant available at -20°C	\$7.89/GJ
Very low-temperature Refrigerant available at -50°C	\$13.11/GJ
Process Water available at desired pressure and 30°C	\$0.067/1000 kg
Waste Water Treatment based on total volume treated	\$56/1000 m^3

Data

All 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. It is suggested that you clearly state this assumption in your written report.

Additionally, the following raw material and product costs should be used:

Raw Material or Product	price
benzene	2.00/gal
ethylene	0.88/kg
ethylbenzene	1.10/kg

Equipment Costs

The equipment costs for the ethylbenzene plant are given below. Each cost is for an individual piece of equipment, including installation. Any pieces of equipment not listed may be considered inexpensive enough to be omitted.

Equipment	Installed Cost in millions of $
Reactor, R-301	0.5
Tower, T-301	1.0
Tower, T-302	0.65
Vessel, V-301	0.1
Any heat exchanger	0.25

Fired heater (H-301) installed cost in dollars:

$$11\times10^{x}$$

where

$$x = 2.5 + 0.8\log_{10} Q$$

where Q is the heat duty in kW

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 24, 2006, at the beginning of class. There will be oral presentations of project results on that day. Oral presentations will continue on April 25, 2006, if we are unable to complete all presentations on April 24, 2006. Oral presentation guidelines will be provided in a separate document.

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

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.

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

Groups

You will work on this project in groups of 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.