Material Balance Project
Styrene Manufacture

We plan to evaluate the economics for a process to manufacture styrene by dehydrogenating ethylbenzene. The pertinent reactions are shown below. Information on reaction equilibrium constants, selectivity, selling prices for reactants and products, and a rough flowsheet are included on the following pages.

Styrene is produced by the reaction

$$\underset{\text{ethylbenzene}}{C_6H_5CH_2CH_3} \underset{\leftarrow}{\longrightarrow} \underset{\text{styrene}}{C_6H_5CHCH_2} + H_2$$

The reaction is reversible and is limited by equilibrium. Reaction occurs at high temperatures (800 K to 950 K) and at low pressures (0.4 bar to 1.4 bar) to shift the equilibrium to the right to favor styrene production. The process uses a proprietary iron catalyst that minimizes side reactions. However, side reactions become significant at higher temperatures. For simplicity, we will assume that the only side reaction is hydrogenolysis of ethylbenzene to produce toluene and methane.

$$\underset{\text{ethylbenzene}}{C_6H_5CH_2CH} + H_2 \rightarrow \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4}$$

The styrene production process is run with a mixture of steam and ethylbenzene. The steam acts as a diluent to shift the reaction equilibrium to the right in favor of styrene and tends to limit side reactions and extend catalyst life. Typical steam to ethylbenzene ratios entering the reactor are 6-12.

The styrene reaction is equilibrium limited. The ethylbenzene-styrene equilibrium constant has the form

$$K_{eq} = \frac{y_S y_H P}{y_{EB}}$$

where, y_S, y_H and y_{EB} are the mole fractions of styrene, hydrogen and ethylbenzene; P is the total pressure in the reactor expressed in bar (1 bar = 100 kPa). The value for the equilibrium constant is only a function of temperature. It is described by the following relationship.

$$\ln K_{eq} = 15.5408 - \frac{14852.6}{T}$$

The temperature units are degrees Kelvin.

You are expected to form small groups and to evaluate the process to determine operating conditions that will produce a maximum profit for a plant that produces 1,000,000,000 lb of styrene per year. You should assume that the reaction temperature range is 800-950 K, the pressure range 0.4-1.4 bar, and the range for the steam to ethylbenzene ratio entering the reactor is 6-12. The primary reaction is equilibrium limited. Assume that this reaction proceeds to 80% of its equilibrium value. The selectivity to the side reaction is listed in Table 1. The flow sheet for the process is provided in Figure 1. No information has been provided about operating costs, so that you should consider profit to be the difference between product value and feedstock cost. Prices and costs are listed in Table 2.

Table 1. Fractional Selectivity for Toluene Formation

Temperature (K)	Fractional Selectivity to Toluene
800	0.01
850	0.03
900	0.06
950	0.13

Table 2. Costs and Selling Prices

Ethylbenzene	$0.250 / lb	Cost
Steam at 800 K	$0.022 / lb	Cost
Styrene	$0.310 / lb	Selling price
Toluene	$0.220 / lb	Selling price
Hydrogen	$0.104 / lb	Selling price
Methane	$0.043 / lb	Selling price
Waste water	$0.002 / lb	Cost

Problem:

You, as a new process engineering team, have been asked to calculate the most profitable mode to operate a styrene production process. You are to determine the operating temperature, pressure, and steam to ethylbenzene ratio. There are a large number of cases that need to be evaluated. You should report the profit (loss) for each case examined and provide stream tables for the best operating conditions found.

You may not use CAD software, but are encouraged to use spreadsheet calculations. You may write your own program if you prefer. If you write a program, any programming language is acceptable. Whether you use a spreadsheet or program, you must turn in hand calculations for one case to demonstrate that the program or spreadsheet was written correctly.

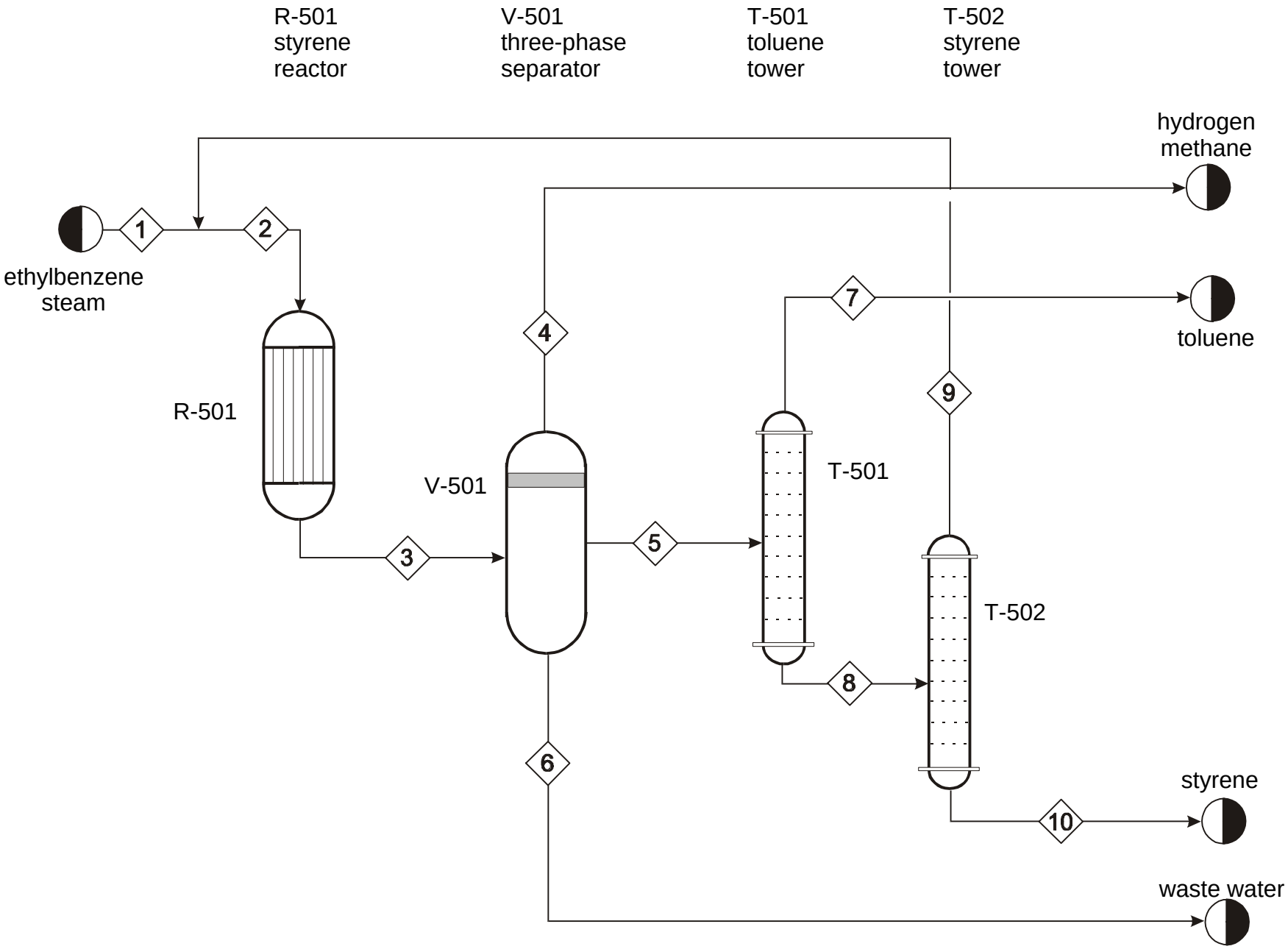

Figure 1: Flowsheet for Styrene Production

Group Formation

A group is to consist of at least 3 and no more than 4 members. No other combinations are acceptable. You are free to make groups by yourselves. When you have formed a group, please write the names of its members on the chart posted on Dr. Kugler's office door. Individuals who do not form their own groups will be assigned to one.

Reports

Each group will be expected to prepare both an oral and a written report recommending best operating conditions. The reports should follow the department's design-report guidelines. Data should be in the form of graphs and tables since this serves both to condense the results and to make them easily understandable. The appendix should include your spreadsheet or computer program and a hand calculation for one representative case.

Report Authors

Although work on a group report can never be divided equitably, only those members of the group making substantial contributions to the final report should be listed as authors.