Material Balances Project
Styrene Manufacture

This project is to evaluate the economics for a process to manufacture styrene by dehydrogenating ethyl benzene. The pertinent reactions are shown below. Information on reaction equilibrium constants, selectivity, selling prices for reactants and products, and a rough flow sheet are included on the following pages.

Styrene is produced by the reaction

$$\underset{\text{ethyl benzene}}{C_6H_5CH_2CH_3} \leftrightarrow \underset{\text{styrene}}{C_6H_5CHCH_2} + H_2$$

The reaction is reversible and is limited by equilibrium. Reaction occurs at high temperatures (800-to-950 K) and at low pressures (0.4-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 ethyl benzene to produce toluene and methane.

$$\underset{\text{ethyl benzene}}{C_6H_5CH_2CH_3} + H_2 \rightarrow \underset{\text{toluene}}{C_6H_5CH_3} + \underset{\text{methane}}{CH_4}$$

The styrene production process is run with a mixture of steam and ethyl benzene. 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-ethyl benzene ratios entering the reactor are 6-12.

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

$$K_{eq} = y_S y_H P / y_{EB}$$

where, y_S, y_H and y_{EB} are the mole fractions of styrene, hydrogen and ethyl benzene; 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.

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

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 1.00 billion 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-ethyl benzene 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 will be provided in a supplemental memo.

Table 1. Fractional Selectivity for Toluene Formation

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

Problem:

You, as a new process engineering team, have been asked to calculate the most profitable mode to operate a styrene production process. Cost data are in Table 2. You are to determine the operating temperature, pressure, and steam-to-ethyl benzene 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.

Table 2. Costs and Selling Prices/lb

Ethyl benzene	$0.50	Cost
Steam at 800 K	$0.044	Cost
Styrene	$0.62	Selling price
Toluene	$0.44	Selling price
Hydrogen	$0.21	Selling price
Methane	$0.086	Selling price
Waste water	$0.004	Cost

You may not use CAD software, but are encouraged to use spreadsheet calculations. You may write your own program if you prefer. Whether you use a spreadsheet or write a program, you must turn in hand calculations for two cases to demonstrate that the program or spreadsheet was written correctly.

Group Formation

A group will typically consist of four students and will be formed by the instructor. To assist in team formation, you should find a partner and put your names on the chart posted on Dr. Kugler's office door. Two-person pairs will then be combined to form four-person groups. Individuals who do not form their own pairs will be assigned to groups.

Reports

Each group will be expected to prepare a written report recommending best operating conditions. The reports should follow the department's design-report guidelines. Data should be in the form

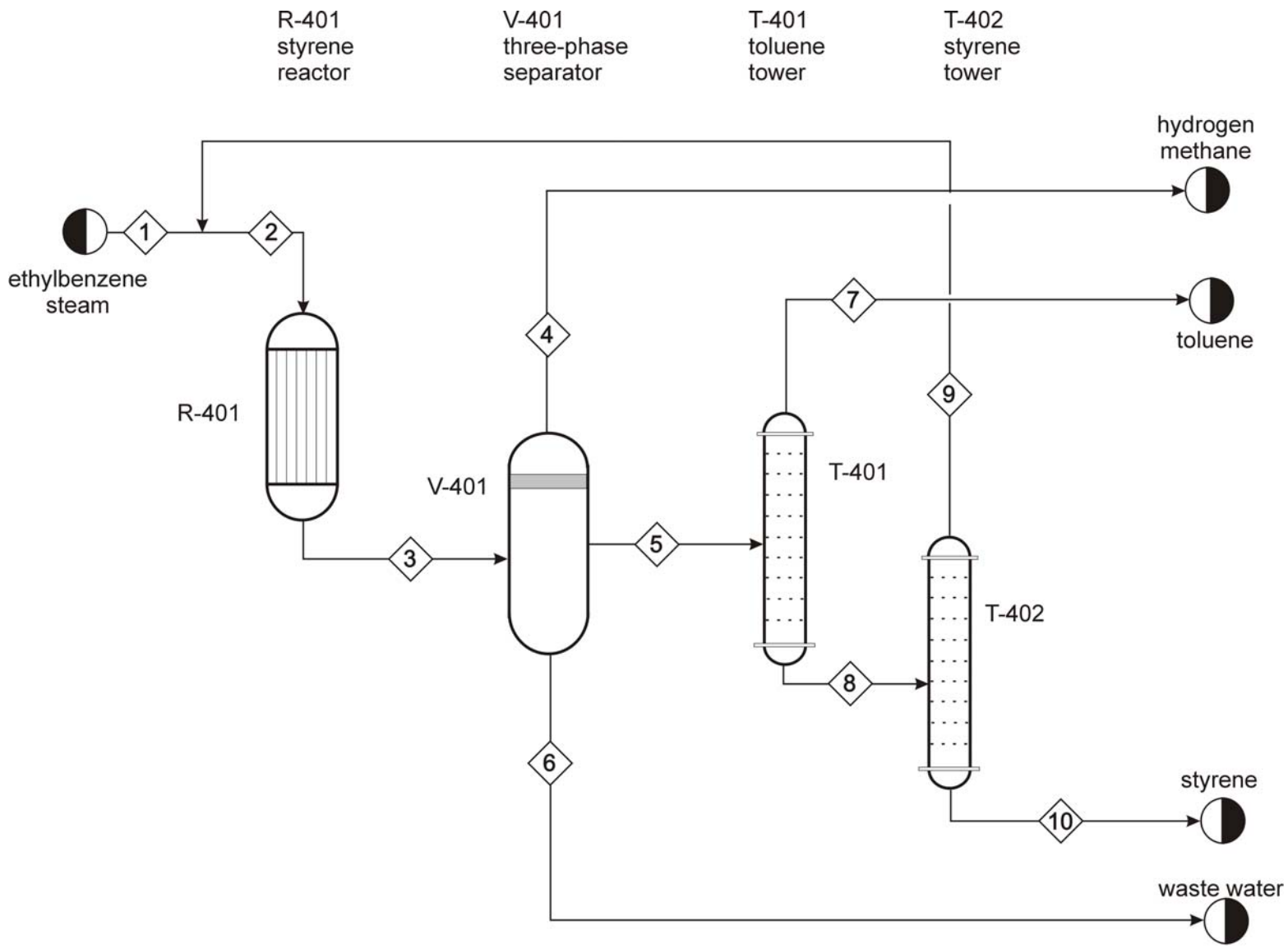

Figure 1: Flowsheet for Styrene Production

of graphs and tables since this serves to both condense the results and make them easily understandable. The appendix should include a copy of this memo, your spreadsheet (or computer program) and two hand calculations.

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.