Material Balances Project
Ethylbenzene

Ethyl benzene (EB) is used as a chemical intermediate in making styrene, the building block for manufacturing polystyrene. It is a major commodity chemical that is produced throughout the world. A byproduct of the process is diethyl benzene (DEB) that is an intermediate in divinyl benzene manufacture. Since the demand for styrene is far greater than the demand for divinyl benzene, the selectivity for our process should favor ethyl benzene production.

Ethyl benzene is produced by coupling ethylene and benzene with an acidic catalyst. Diethyl benzene forms when ethylene reacts with ethyl benzene. The formation of multiply-substituted benzenes is limited by running the reaction with a large excess of benzene. The reactions that produce EB and DEB are

$$C_6H_6 + C_2H_4 \rightarrow C_6H_5C_2H_5 \qquad \zeta_1$$

$$C_6H_6 + 2C_2H_4 \rightarrow C_6H_4(C_2H_5)_2 \qquad \zeta_2$$

where ζ_ι is the extent of reaction. The selectivity of these reactions is determined by the feed ratio and processing conditions. A simplified process flow diagram is shown in the appended figure.

Process Description

Fresh benzene (Stream 1) and ethylene (Stream 2) are combined with a recycle stream containing unreacted benzene and a small amount of ethyl benzene. The combined stream is fed to a reactor where all of the ethylene in the feed reacts. The reactor effluent (Stream 4) is cooled so that most of the benzene, ethyl benzene, and diethyl benzene condenses. An ethane impurity from the ethylene feed as well as some benzene and ethyl benzene vapor are purged from the process and used as fuel gas. The condensed liquid is fed to the first distillation column. A high purity benzene stream is removed from the top of the column and recycled. The bottoms from the first column are sent to a second distillation column. The second column produces high-purity ethyl benzene in the top stream and diethyl benzene in the bottom. Data on the composition of these streams are provided in a following section.

Additional Process Information

Stream 1	– Assume that benzene is pure.
Stream 2	– The ethylene feed contains 7.0 mol% ethane as an impurity. Ethane does not react but moves through the process as an inert gas until it is purged in Stream 5.
Stream 3	– Benzene-to-ethylene molar ratio is adjusted to control reaction selectivity. Use a 10:1 ratio when making hand calculation.
R-301	– The limiting reactant achieves 100% conversion. Reaction selectivity is determined by B_3/E_3 ratio. See relationship below.
Stream 5	– Fuel gas composition is 40 mol% ethane, 55 mol% benzene and 5 mol% ethyl benzene.
Stream 7	– Recycle stream composition is 99.2 mol% benzene and 0.8 mol% ethyl benzene.

Stream 9 – Overhead stream composition is 99.6 mol% ethyl benzene, 0.4 mol% benzene.
Stream 10 – Bottoms stream composition is 90 mol% diethyl benzene, 10 mol% ethyl benzene.

Reaction Information

The selectivity for ethyl benzene production is a function of benzene-to-ethylene ratio. This relationship is expressed as

$$\frac{\zeta_2}{\zeta_1} = \left(\frac{E_3}{B_3}\right)^{1.2}$$

However, the size of T-301 limits the B_3/E_3 ratio to a maximum value of 12.

Operating Costs

Much of the expense in manufacturing ethyl benzene is associated with utility costs like compressing gases to reaction pressure and evaporating liquids for separation in distillation towers. These costs cannot be estimated well in a first chemical engineering course. Therefore, utility costs may be ignored this semester. The difference between product price and feedstock cost should be called revenue. It should not be called profit, since operating and other expenses have not been included.

ethylene cost = $ 0.77 /kg
benzene cost = $ 1.22 /kg
EB price = $ 1.54 /kg
DEB price = $ 0.76 /kg
Fuel gas value = $ 0.54 /kg

Problem

You, the engineering team, are to optimize the operation of the EB process in order to produce 100,000 metric-tons/yr (100,000,000 kg/yr). Your goal is to minimize operating costs and maximize revenue. You are constrained by the selectivity of the reaction and by the size of T-301 used for separating and recycling excess benzene.

Group Formation

A design group is to consist of two members. You are encouraged to make groups by yourselves. When you have formed a group, please turn in the names of group members to Dr. Kugler. He will combine groups to make 3- or 4-person design teams. A list of design teams will be provided on November 12.

Computations

You are expected to use a spreadsheet for material balance and cost calculations. The first step should be solving the material balance by hand calculations. Use a basis of n_2 = 100 kmol/h and the reactor-feed ratio of B_3/E_3 = 10. After completing the hand calculation, set up the spreadsheet to do the material balance when you specify B_3/E_3 ratio. Copy results into a stream table. These first steps, including pencil-written hand calculations, should be included as an appendix to your report to demonstrate that calculations were done correctly.

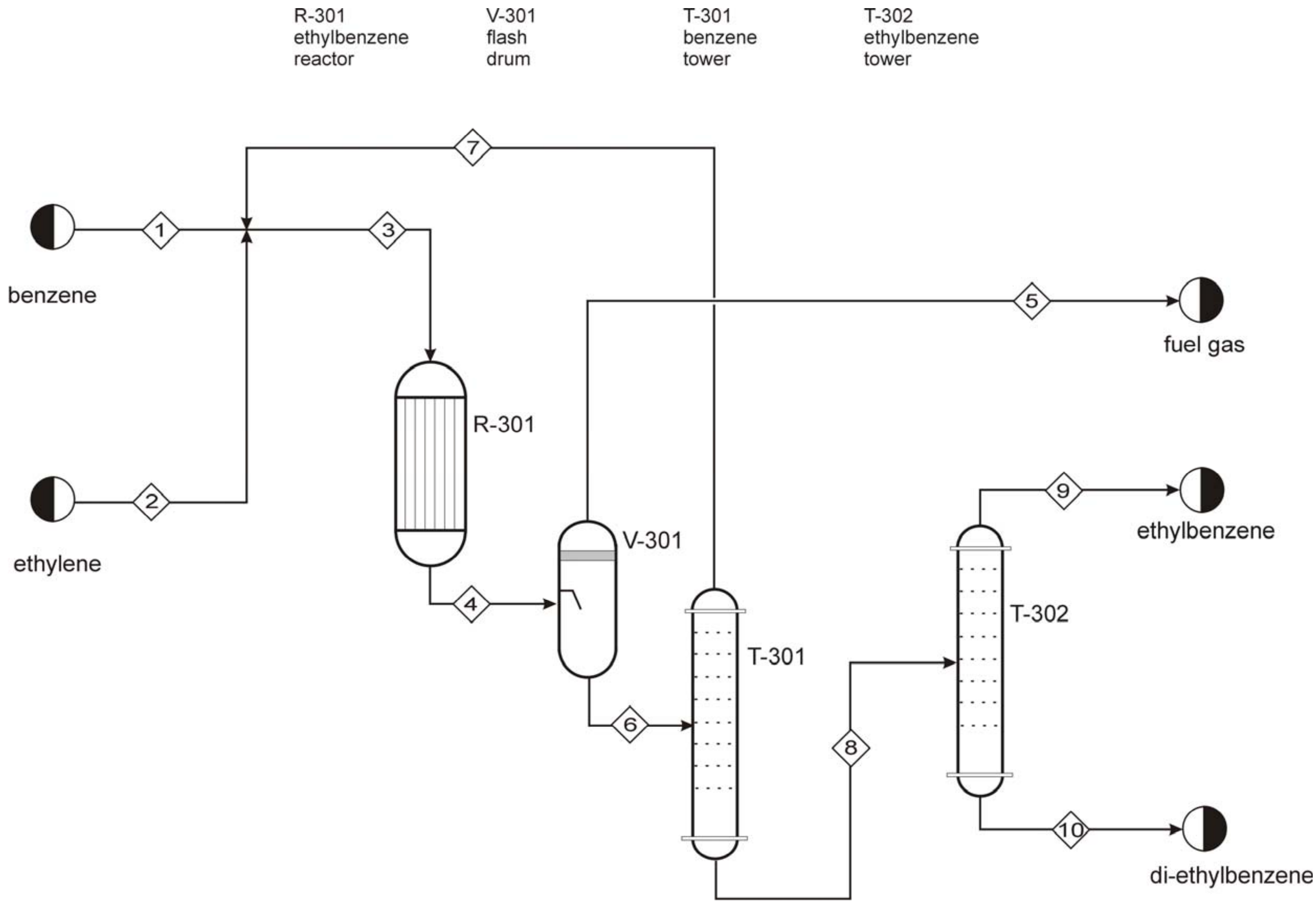
After producing a stream table on your spreadsheet using kmol units, convert kmol units to mass on a second stream table, then scale so that EB meets production goal. Profit or loss for selected operating conditions can be calculated from scaled-stream-table data.

Reports

Each team will be expected to prepare a written report recommending the best operating procedures for the EB process. This report is due at 3:00 PM, Wednesday, December 7. The report should follow the Department's design-report guidelines. Data should be in the form of graphs and tables, since this serves both to condense results and make them easily understandable. The appendix should include your spreadsheet and a hand calculation of the 10/1 case.

Report Authors

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



Unit 300: Ethylbenzene Process