Styrene Manufacturing Homework/Project

Notes:
1. The project report should be your own (group) work. In case of plagiarism, the report will not be considered for any credit.
2. You can use any process simulator of your choice to estimate any component properties or to compute reaction/separation calculations
3. The final project report is due 16/04/2020
4. Even though it is a group project, individually you are responsible for the entire content of the project. In other words, during viva, you will be asked questions about any part of the project report, irrespective of whether you have worked on it or not.

Styrene (also called styrene monomer) is an important petrochemical product. It is predominantly used to make polystyrene which finds multitude of applications. One of the most common way of producing styrene is dehydrogenation of ethylbenzene ($>$ 90% worldwide production). In fact, manufacture of styrene from ethylbenzene accounts for more than 50% of the consumption of commercial benzene. A typical styrene plant starts with benzene and ethylene as feeds to first produce ethylbenzene, which is then dehydrogenated to get styrene. However, for this project, we will consider only the dehydrogenation part, starting with ethylbenzene. The following significant reactions take place.

$$Ethylbenzene \rightleftharpoons Styrene + Hydrogen \tag{1}$$
$$Ethylbenzene \rightarrow Benzene + Ethylene \tag{2}$$
$$Ethylbenzene + Hydrogen \rightarrow Toluene + Methane \tag{3}$$

The primary reaction is endothermic (as most of the dehydrogenation reactions are) and it typically equilibrium limited. The reaction is carried out in the presence of steam which serves three purposes (can you guess them?). The reaction temperature is 550-680 C and typically low pressure operation is favoured. Reaction kinetic and thermodynamic data is given below:

$$r_{1,f} = 0.044exp\left(-\frac{90981}{RT}\right)p_{ethylbenzene} \tag{4}$$
$$r_{1,b} = 6\times10^{-8}exp\left(-\frac{61127}{RT}\right)p_{styrene}p_{hydrogen} \tag{5}$$
$$r_{2} = 27100exp\left(-\frac{207989}{RT}\right)p_{ethylbenzene} \tag{6}$$
$$r_{3} = 6.484\times10^{-7}exp\left(-\frac{91515}{RT}\right)p_{ethylbenzene}p_{hydrogen} \tag{7}$$

r_i is the rate of reaction in kmol/m^3-reactor/s, p_i is partial pressure of component i in Pa, R = 8.314J/mol/K.

We are interested in pursueing conceptual process design for producing 120 kmol/h of polymer-grade styrene monomer (99.95% purity). Note that styrene product has a tendency to spontaneously polymerize at high temperature. Therefore, it is required that styrene product temperature should be maintained less than 125 C. Normal boiling point of styrene is 145 C, so the final distillation should be run under vacuum. Raw material ethylbenzene contains small impurities of benzene (1% of EB) and Toluene (1% of EB). Steam to hydrocarbon ratio of 6:1 to 12:1 is common.

Over the course of the semester, we will apply hierarchical design methodology to this example. Specifically,

Task 1. We will first generate product distribution as a function of conversion. Lets consider that these reactions are carried out in a batch reactor of 30 m^3. Consider that initially 100 mol feed is charged. The reactions are carried out at 560 C and initial pressure of 300 kPa. Steam to hydroacrbon ratio of 12:1 is used. Using the kinetic rate equations given above, write Matlab codes to simulate the batch reactor composition dynamics. Using this data, obtain approximate functional forms of the following relationships

- selectivity of styrene and ethylbenzene conversion
- selectivity of benzene (or toluene) and ethylbenzene conversion

Task 2. Perform level 2 design and compute economic potential. Plot variation of economic potential as a function of key design variables. You can use the following data for calculations.

Component	NBP (C)	Price ($/kmol)	Fuel value (MMBtu/kmol)
Styrene	145	23	N/A
Ethylbenzene	136	16	N/A
Benzene	80	9	1.41
Toluene	111	8.5	1.68
Hydrogen	-253	N/A	0.123
Methane	-161	N/A	0.383
Ethylene	-104	N/A	0.596
Steam	100	0.07	N/A
Fuel	N/A	$4/MMBtu	N/A

Task 3. Perform level 3 design and compute economic potential. Plot variation of economic potential as a function of key design variables.

Task 4. Perform level 4 design. Carry out linear material balance and identify key decision variables and associated trade offs.

Task 5. Simulate the flowsheet at level 4 design using any process simulator.

Task 6. Identify heating and cooling requirements of the process. Perform level 5 design.

Task 7. Simulate the flowsheet at level 5 design using any process simulator.

Task 8. Perform economic analysis and assess profitability of the designed process.

In addition to these tasks, you can evaluate and compare multiple design alternatives to present a convincing final design.