Problem 1

Is it possible to use a CSTR or PFR reactor in place of the batch reactor in Example 6.3 from the course to get similar of better results in continuous? Simulate both reactors to justify your answer.

Problem 2

Consider the following system of gas-phase reactions that was already studied in problem set 6:

$A \rightarrow X$ with $r_1 = 0.004 \cdot C_A^{0.5}$ mol/(L·min)

$A \rightarrow B$ with $r_2 = 0.3 \cdot C_A$ mol/(L·min)

$A \rightarrow Y$ with $r_3 = 0.25 \cdot C_A^2$ mol/(L·min)

B is the desired product, and X and Y are foul pollutants that are expensive to get rid of. The specific reaction rates are at 27°C. The reaction system is to be operated at 27°C and 4 atm. Pure A enters the system at a volumetric flow rate of 10 L/min.

1. Suppose that E_1 = 20000 cal/mol, E_2 = 10000 cal/mol, and E_3 = 30000 cal/mol. What temperature would you recommend for a single CSTR with a mean residence time of 10 min and an entering concentration of A of 0.1 mol/dm³?
2. If you could vary the pressure between 1 and 100 atm, what pressure would you choose?

Problem 3

The following reactions

$$A \overset{k_1, K_1}{\longleftrightarrow} D$$

$$A \overset{k_2, K_2}{\longleftrightarrow} U$$

take place in a batch reactor with the following additional information:

$k_1 = 1.0\ \text{min}^{-1}$, $K_1 = 10$

$k_2 = 100\ \text{min}^{-1}$, $K_2 = 1.5$

$C_{A0} = 1\ \text{mol/L}$

1. Plot and analyze conversion and the concentrations of A, D, and U as a function of time. When would you stop the reaction to maximize the concentration of D? Describe what you find.

2. When does the maximum concentration of U occur?
3. What are the equilibrium concentrations of A, D, and U?
4. What would be the exit concentrations from a CSTR with a mean residence time of 1.0 min? Of 10.0 min? Of 100 min?