Problem 1

Consider the following system of gas-phase reactions:

$A \rightarrow X$ 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) Sketch the instantaneous selectivity $s_{B/XY} = R_B/(R_X+RY)$) as a function of the concentration of C_A.
2) Consider a series of reactors. What should be the volume of the first reactor?
3) What are the effluent concentrations of A, B, X, and Y from the first reactor?
4) What is the conversion of A in the first reactor?
5) If 99% conversion of A is desired, what reaction scheme and reactor sizes should you use to maximize $S_{B/XY}$?

Problem 2

We carry out out the following chemical reactions in gas phase :

$A + B \rightarrow U \;\; r_1 = k_1 C_A^2 C_B$ with $k_1 = 3$ L^2/mol^2·s

$A + B \rightarrow D \;\; r_2 = k_2 C_A C_B^2$ with $k_2 = 2$ L^2/mol^2·s

We want to compare the overall selectivities of the desired product D relative to the undesired product U (F_D/F_U) for a membrane tubular reactor and a conventional PFR reactor. The reactor volume is 50 L, and the total incoming concentration in the reactor is 0.8 mol/L, with the molar flows of incoming A and B both at 4 mol/s. For the PFR, B enters with A. For the membrane tubular reactor, we want to compare the situation where A is dosed through the membrane, with that where B is dosed through the membrane. The molar flow rate of species i crossing the membrane per unit volume is uniform over the entire reactor and is given by $R_{iM} = F_{i0}/Vtot$.

Problem 3

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