Problem 1. Qualitative Reactor Design for Multiple Reactions

We seek to maximize the **selectivity** for the desired product D. For each of the following networks explain:

i) What type of flow reactor is optimal: a CSTR, a PFR, or a recycle reactor.

ii) Whether we want a small, intermediate, or large space time.

iii) Whether we want a low, intermediate, or high inlet concentration of A.

iv) Whether we want to introduce diluents in the feed.

v) Whether we want a low, intermediate, or high inlet pressure.

vi) Whether we want a low, intermediate, or high operating temperature.

a. The elementary gas-phase reaction sequence:

$$2\ \mathrm{A} \xrightarrow{k_1} \mathrm{D}$$
$$\mathrm{A} + \mathrm{D} \xrightarrow{k_2} \mathrm{U}$$

with $E_1 < E_2$.

b. The gas-phase reaction sequence:

$$\mathrm{A} \xrightarrow{k_1} \mathrm{U} \quad -r_\mathrm{A} = k_1 C_\mathrm{A}^{1/2} \text{ with } k_1 = 4.0 \times 10^{-3} e^{-5000\ \mathrm{K}/T}$$
$$\mathrm{A} \xrightarrow{k_2} \mathrm{D} \quad -r_\mathrm{A} = k_2 C_\mathrm{A} \text{ with } k_2 = 3.0 \times 10^{-1} e^{-5000\ \mathrm{K}/T}$$
$$\mathrm{A} \xrightarrow{k_3} \mathrm{W} \quad -r_\mathrm{A} = k_3 C_\mathrm{A}^{2} \text{ with } k_3 = 2.5 \times 10^{-1} e^{-5000\ \mathrm{K}/T}$$

Problem 2. Reactions in Series

The elementary liquid-phase-series reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ is conducted in a 500.-L reactor fed pure A with a concentration of 1.60 M. The desired product is B, and separation of the undesired product C is very difficult and costly. The following data are available for the rate constants at 100.00 °C: $k_1 = 5.00\times10^{-1}\ h^{-1}$ and $k_2 = 1.00\times10^{-2}\ h^{-1}$.

a. Use of a PFR

i. What is the optimal volumetric flow rate (in L/h) to maximize **concentration** of B?

ii. What is the conversion of A when the PFR is operated at this optimum?

iii.. What are the concentrations of B and C (in M) in the effluent?

iv. What are the values of the selectivity $\tilde{S}_{B/C}$ and the yield $\tilde{Y}_B$?

b. Use of a CSTR

Repeat part a based on a CSTR. Compare your answers for a CSTR *vs.* a PFR.

Problem 3. Parallel Reactions

Consider the following system of gas-phase reactions:

$A \xrightarrow{k_1} X$	$r_X = k_1$	k_1 = 5.0×10^{-4} M/min
$A \xrightarrow{k_2} B$	$r_B = k_2 C_A$	k_2 = 1.0 min^{-1}
$A \xrightarrow{k_3} Y$	$r_Y = k_3 C_A^{\ 2}$	k_3 = 60. M^{-1}-min^{-1}

B is the desired product; X and Y are foul pollutants that are expensive to dispose.

a. What type of reactor minimizes the selectivity for X, $S_{X/B}$? What type of reactor minimizes the selectivity for Y, $S_{Y/B}$?

b. We wish to maximize the production of B with a conversion of A of 90.% using a CSTR and a PFR placed in series with a 6.1×10^{-3} M feed of pure A at 1.0 mol/min.

   i. Based on minimizing an overall selectivity for the foul pollutants, $S_{overall} \equiv S_{X/B} + S_{Y/B}$, how should the reactor network be configured?

   ii. What is the conversion for the first reactor based on an optimal design of $S_{X/B} = S_{Y/B}$?

   iii. What are the volumes in (L) for the CSTR and PFR.

Problem 4. Complex Reaction

Create a Jupyter notebook or Excel file to answer the following question.

Terephthalic acid (TPA) finds extensive use in the manufacture of synthetic fibers (e.g., Dacron) and as an intermediate for polyester films (e.g., Mylar). The formation of potassium terephthalate from potassium benzoate was studied using a tubular reactor [Ind. Eng. Chem. Res., 26, 1691 (1987)].

It was found that the intermediates (primarily K-phthalates) formed from the dissociation of K-benzoate over a CdCl2 catalyst reacted with K-terephthalate in an autocatalytic reaction step

$$A \overset{k_1}{\rightarrow} R \overset{k_2}{\rightarrow} S \ (series)$$

$$R + S \overset{k_3}{\rightarrow} 2S \ (autocatalytic)$$

where A = K-benzoate, R = lumped intermediates (K-phthalates, Kisophthalates, and K-benzenecarboxylates), and S = K-terephthalate.

Pure A is charged to the reactor at a pressure of 110 kPa. The specific reaction rates at 410 ◦C are $k_1 = 1.08 \times 10^{-3}\ s^{-1}$ with E_1 = 42.6 kcal/mol, $k_2 = 1.19 \times 10^{-3}\ s^{-1}$ with E_2 = 48.6 kcal/mol, and $k_3 = 1.59 \times 10^{-3}$ L/mol/s with E_3 = 32 kcal/mol.

(a) Plot and analyze the concentrations of A, R, and S as a function of time in a batch reactor at 410 ◦C, noting the value when the maximum in R occurs.

(b) Repeat (a) for temperatures of 430 ◦C and 390 ◦C.

(c) What would be the exit concentrations from a CSTR operated at 410 ◦C and a space time of 1200 s?

- Use scipy.optimize.root---or Excel Solver