CH7003 – Practice Problem Set 1 (AY2018)
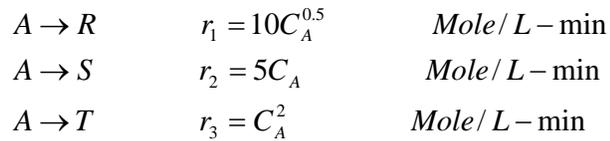
1. The following parallel reactions are known to occur (C_A is concentration of A):

$$A \rightarrow R \qquad r_1 = 10C_A^{0.5} \qquad Mole/L - min$$
$$A \rightarrow S \qquad r_2 = 5C_A \qquad Mole/L - min$$
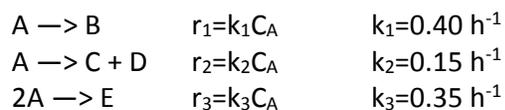$$A \rightarrow T \qquad r_3 = C_A^2 \qquad Mole/L - min$$

The feed concentration is C_{A0}=10 mole/L. The volumetric flow rate is 1000L/min. T is the desired product.

(a) Find the optimum <u>selectivity</u> and the <u>conversion</u> at that point. What is the preferred reactor (PF or CSTR)?
(b) Find the optimum <u>yield</u> and the conversion at that yield. (Please use a graph paper)
(c) Express r in terms of C_A and <u>describe</u> how you can graphically determine the volume of reactor needed.

2. CSTR and PFTR reactors are used in series for the reaction A→ 4B, r = kC_A^2. The feed consists of 90 mol% A and 10mol% inert gas. A, B and the inert gas can be regarded as ideal gases. v_0 = 5 liter/min, k = 1 liter/mole min, and C_{A0} = 2 moles/liter. If the conversion after the first reactor is set at 50% and after the second reactor is set at 80%, how should you arrange the reactors to minimize the reactors' total volume and what should be the sizes of these two reactors?

3. A 100-Litre CSTR is used for a reaction that follows a 2nd-order rate law:

$$-r_a = kC_{A0}^2(1-X)^2$$

where X is the conversion and C_{A0} is the inlet concentration of the limiting reactant. A conversion of 75% is achieved in the CSTR. A PFR of the same volume is added in series to the CSTR to increase the conversion. Should it be added before of after the CSTR? What is the final conversion?

4. Three reactions occur in an isothermal batch reactor:

$$A \longrightarrow B \qquad r_1=k_1C_A \qquad k_1=0.40 \ h^{-1}$$
$$A \longrightarrow C + D \qquad r_2=k_2C_A \qquad k_2=0.15 \ h^{-1}$$
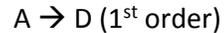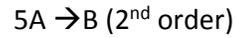$$2A \longrightarrow E \qquad r_3=k_3C_A \qquad k_3=0.35 \ h^{-1}$$

Given the following initial concentrations, what is reaction time needed for 90% conversion?

C_{A0}= 10 mol/L C_{B0}= 0 mol/L C_{C0}= 0.8 mol/L C_{D0}= 0.8 mol/L C_{E0}= 0.5 mol/L

5.   Provide explanations backed by illustrations for the following scenarios.

a) Two gas-phase reactions take place in an isothermal plug flow reactor:

$5A \rightarrow B$ (2nd order)
$A \rightarrow D$ (1st order)

Two other gas-phase reactions take place in an identical PFR:

$A \rightarrow C$ (2nd order)
$A \rightarrow E$ (1st order)
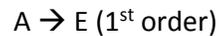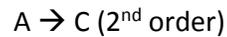
If the rate constants for the 2nd order reactions are the same and the rate constants for the 1st order reactions are the same, which selectivity is higher, ie $5F_B/F_D$ or F_C/F_E.

b) An isothermal batch reactor is used to carry out a 1st order reaction in the aqueous phase (500 L of liquid at start). The time to reach 90% conversion is 4 hr. After 1 hr, a valve was opened by mistake and 500 L of water flow into the reactor before it is closed. What will be the total reaction time to obtain 90% conversion now?

c) A piston cylinder system contains CaO (s), $CaCO_3$ (s), CO_2 and N_2 in equilibrium at 850K. A syringe is used t remove 25% of the gas phase. The piston remains isothermal at constant temperature. Explain what happens to the solid phases.