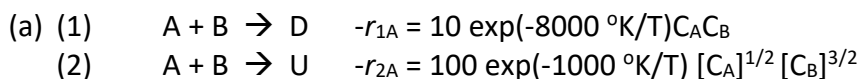


## Assignment 4 - Solutions

1. For each of the following sets of reactions, describe reactor system and conditions to maximize the selectivity to D. The rates are in mol/(dm<sup>3</sup>.s) and concentrations are in mol/dm<sup>3</sup>. [6 Marks total]



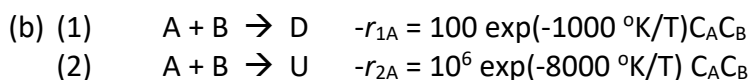
$$S_{D/U} = \frac{r_D}{r_U} = \frac{10e^{-\frac{8000}{T}} C_A C_B}{100e^{-\frac{1000}{T}} C_A^{1/2} C_B^{3/2}} = \frac{0.1e^{-\frac{7000}{T}} C_A^{1/2}}{C_B^{1/2}}$$

[1 Mark] Reactor: Series of small CSTR with A flowing to the first CSTR and B added to each CSTR

PFR with A entering at the inlet, B as side streams

Semibatch reactor with A taken whole and B added slowly.

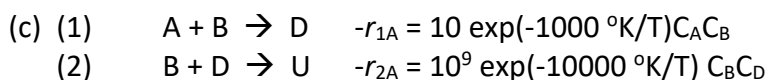
[1 Mark] Temperature: operate at high temperature



$$S_{D/U} = \frac{r_D}{r_U} = \frac{100e^{-\frac{1000}{T}} C_A C_B}{10^6 e^{-\frac{8000}{T}} C_A C_B} = 10^{-4} e^{\frac{7000}{T}}$$

[1 Mark] Reactor: Any reactor type will do.

[1 Mark] Temperature: operate at low temperature



$$S_{D/U} = \frac{r_D}{r_U} = \frac{10e^{-\frac{1000}{T}} C_A C_B}{10^9 e^{-\frac{10000}{T}} C_B C_D} = 10^{-4} e^{\frac{7000}{T}} \frac{C_A}{C_D}$$

[1 Mark] Reactor: PFR with high concentration of A (high pressure, no inert)

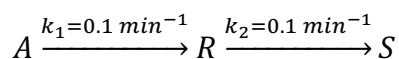
Remove D if possible; B can be introduced in any fashion.

Batch reactor with high concentration of A

Remove D if possible; B can be introduced in any fashion.

[1 Mark] Temperature: Operate at low temperature

2. Under certain conditions, A decomposes as follows



R is to be produced from 1000 liter/hr of feed in which  $C_{A0} = 1 \text{ mol/liter}$ ,  $C_{R0} = C_{S0} = 0$ .

(a) What size of plug flow reactor will maximize the concentration of R, and what is that concentration in the effluent stream from this reactor? [4 Marks total]

$$\tau_{max} = \frac{\ln(k_2/k_1)}{k_2 - k_1}$$

$$\text{For } k_2 = k_1, \tau_{max} = \frac{1}{k_1} = 10 \text{ min. [2 Marks]}$$

$$\frac{C_{R,max}}{C_{A0}} = \left(\frac{k_1}{k_2}\right)^{k_2/(k_2-k_1)}$$

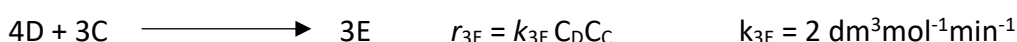
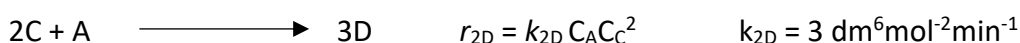
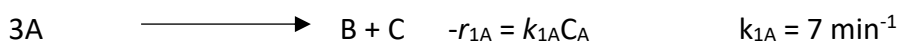
$$\text{For } k_2 = k_1, C_{R,max} = \frac{1}{e} = 0.368 C_{A0} = 0.368 \text{ mol/liter. [2 Marks]}$$

(b) What size of mixed flow reactor will maximize the concentration of R, and what is  $C_{R,max}$  in the effluent stream from this reactor? [4 Marks total]

$$\text{[2 Marks]} \tau_{max} = \frac{1}{\sqrt{k_1 k_2}} = 10 \text{ min}$$

$$\text{[2 Marks]} C_{R,max} = \frac{k_1 C_{A0}}{2\sqrt{k_1 k_2} + k_1 + k_2} = 0.25 \text{ mol/lit}$$

3. The following liquid-phase reactions were carried out in a CSTR at 325 K: [26 Marks total]



The concentrations measured inside the reactor were  $C_A = 0.1$ ,  $C_B = 0.93$ ,  $C_C = 0.51$ , and  $C_D = 0.049$  all in  $\text{mol/dm}^3$ .

(a) What are the values of  $r_{1A}$ ,  $r_{2A}$ , and  $r_{3A}$ ?

$$r_{1A} = -k_{1A} C_A = -7 \cdot 0.1 = -0.7 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_{2A} = -r_{2D} / 3 = -k_{2D} C_A C_C^2 / 3 = -3 \cdot 0.1 \cdot (0.51)^2 / 3 = -0.026 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_{3A} = 0 \text{ [1 Mark]}$$

(b) What are the values of  $r_{1B}$ ,  $r_{2B}$ , and  $r_{3B}$ ?

$$r_{1B} = -r_{1A} / 3 = 0.233 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_{2B} = 0 \text{ [1 Mark]}$$

$$r_{3B} = 0 \text{ [1 Mark]}$$

(c) What are the values of  $r_{1C}$ ,  $r_{2C}$ , and  $r_{3C}$ ?

$$r_{1C} = -r_{1A}/3 = 0.233 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_{2C} = -2/3 r_{2D} = -0.052 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_{3C} = -r_{3E} = k_{3E} C_D C_C = -2 * 0.049 * 0.51 = -0.05 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

(d) What are the values of  $r_{1D}$ ,  $r_{2D}$ , and  $r_{3D}$ ?

$$r_{1D} = 0 \text{ [1 Mark]}$$

$$r_{2D} = 0.078 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_{3D} = -4/3 r_{3E} = -4/3 * 2 * 0.049 * 0.51 = -0.0667 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

(e) What are the values of  $r_{1E}$ ,  $r_{2E}$ , and  $r_{3E}$ ?

$$r_{1E} = 0 \text{ [1 Mark]}$$

$$r_{2E} = 0 \text{ [1 Mark]}$$

$$r_{3E} = 0.05 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

(f) What are the net rates of formation of species A, B, C, D and E?

$$r_A = -0.726 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_B = 0.233 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_C = 0.131 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_D = 0.0113 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

$$r_E = 0.05 \text{ mol}/(\text{dm}^3 \cdot \text{min}) \text{ [1 Mark]}$$

(g) The entering volumetric flow rate is  $100 \text{ dm}^3/\text{min}$  and the entering concentration of A is  $3 \text{ mol/liter}$ . What is the CSTR reactor volume?

$$\frac{V}{v_0} = \frac{C_{A0} - C_A}{-r_A}; V = 400 \text{ dm}^3. \text{ [1 Mark]}$$

(h) What are the exit molar flow rates from the CSTR of volume obtained in (g)?

$$F_A = v_0 C_A = 10 \text{ mol/min} \text{ [1 Mark]}$$

$$F_B = v_0 C_B = 93 \text{ mol/min} \text{ [1 Mark]}$$

$$F_C = v_0 C_C = 51 \text{ mol/min} \text{ [1 Mark]}$$

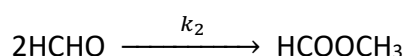
$$F_D = v_0 C_D = 4.9 \text{ mol/min} \text{ [1 Mark]}$$

$$C_E \text{ is not known. But we know that } \frac{V}{v_0} = \frac{C_{E0} - C_E}{-r_E} = 4$$

$$\text{Solving for } C_E, C_E = 0.2 \text{ mol}/\text{dm}^3$$

$$F_E = v_0 C_E = 20 \text{ mol/min. [1 Mark]}$$

4. The complex reactions involved in the oxidation of formaldehyde to formic acid over a Vanadium titanium oxide catalyst are shown below. Each reaction follows an elementary rate law:



Let A = HCHO, B = O<sub>2</sub>, C = HCOOH, D = HCOOCH<sub>3</sub>, E = CO, W = H<sub>2</sub>O and G = CH<sub>3</sub>OH.

The entering flow rates are  $F_{A0} = 10$  mol/s and  $F_{B0} = 5$  mol/s, and  $v_0 = 100$  dm<sup>3</sup>/s. At a total entering concentration  $C_{T0} = 0.147$  mol/dm<sup>3</sup>, the suggested reactor volume is 1000 dm<sup>3</sup>.

Data available:

At 300 K,

$$k_1 = 0.014 \text{ (dm}^3\text{/mol)}^{1/2} \text{ s}^{-1}.$$

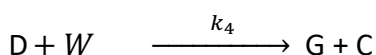
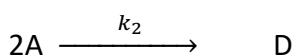
$$k_2 = 0.007 \text{ dm}^3\text{/(mol.s)}$$

$$k_3 = 0.014 \text{ s}^{-1}$$

$$k_4 = 0.45 \text{ dm}^3\text{/(mol.s)}$$

- Plot the molar flow rates of each species along the volume (length) of the reactor on the same figure.
- Plot and analyze  $\tilde{Y}_C$ ,  $\tilde{S}_{A/E}$ ,  $\tilde{S}_{C/D}$  and  $\tilde{S}_{D/G}$  along the length of the reactor. Find volume at which maximum occur, if any.

**Solution: [10 marks]**



$$r_A = -k_1 C_A C_B^{1/2} - k_2 C_A^2$$

$$r_B = -\frac{1}{2} k_1 C_A C_B^{1/2}$$

$$r_C = k_1 C_A C_B^{1/2} - k_3 C_C + k_4 C_D C_W$$

$$r_D = \frac{1}{2} k_2 C_A^2 - k_4 C_D C_W$$

$$r_E = k_3 C_C$$

$$r_G = k_4 C_D C_W$$

$$r_W = k_3 C_C - k_4 C_D C_W$$

$$\frac{dF_i}{dV} = r_i \text{ and } C_i = C_{T0} \frac{F_i}{F_T} \text{ where } F_T = \sum F_i$$

Solve the ODEs numerically in Matlab.