Assignment 4
(Submission deadline-11 Sept 2020, 5 PM)

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^3.s) and concentrations are in mol/dm^3.

(a) (1) A + B → D $-r_{1A} = 10 \exp(-8000\ ^{o}K/T)C_AC_B$
(2) A + B → U $-r_{2A} = 100 \exp(-1000\ ^{o}K/T)\ [C_A]^{1/2}\ [C_B]^{3/2}$

(b) (1) A + B → D $-r_{1A} = 100 \exp(-1000\ ^{o}K/T)C_AC_B$
(2) A + B → U $-r_{2A} = 10^6 \exp(-8000\ ^{o}K/T)\ C_AC_B$

(c) (1) A + B → D $-r_{1A} = 10 \exp(-1000\ ^{o}K/T)C_AC_B$
(2) B + D → U $-r_{2A} = 10^9 \exp(-10000\ ^{o}K/T)\ C_BC_D$

2. Under certain conditions, A decomposes as follows

$$A \xrightarrow{k_1=0.1\ min^{-1}} R \xrightarrow{k_2=0.1\ min^{-1}} S$$

R is to be produced from 1000 liter/hr of feed in which C_{A0} = 1 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?
(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?

3. The following liquid-phase reactions were carried out in a CSTR at 325 K:

$3A \longrightarrow B + C$		$-r_{1A} = k_{1A}C_A$	k_{1A} = 7 min^{-1}
$2C + A \longrightarrow 3D$		$r_{2D} = k_{2D}\, C_AC_C^2$	k_{2D} = 3 dm^{6}mol^{-2}min^{-1}
$4D + 3C \longrightarrow 3E$		$r_{3E} = k_{3E}\, C_DC_C$	k_{2D} = 2 dm^{3}mol^{-1}min^{-1}

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 mol/dm^3.

(a) What are the values of r_{1A}, r_{2A}, and r_{3A}?
(b) What are the values of r_{1B}, r_{2B}, and r_{3B}?
(c) What are the values of r_{1C}, r_{2C}, and r_{3C}?
(d) What are the values of r_{1D}, r_{2D}, and r_{3D}?
(e) What are the values of r_{1E}, r_{2E}, and r_{3E}?
(f) What are the net rates of formation of species A, B, C, D and E?
(g) The entering volumetric flow rate is 100 dm^3/min and the entering concentration of A is 3 mol/liter. What is the CSTR reactor volume?
(h) What are the exit molar flow rates from the CSTR of volume obtained in (*g*)?

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:

$$HCHO + \tfrac{1}{2}\,O_2 \xrightarrow{k_1} HCOOH \xrightarrow{k_3} CO + H_2O$$

$$2HCHO \xrightarrow{k_2} HCOOCH_3$$

$$HCOOCH_3 \xrightarrow{k_4} CH_3OH + HCOOH$$

Let A = HCHO, B = O_2, C = HCOOH, D = $HCOOCH_3$, E = CO, W = H_2O and G = CH_3OH.
The entering flow rates are F_{A0} = 10 mol/s and F_{B0} = 5 mol/s, and v_0 = 100 dm^3/s. At a total entering concentration C_{T0} = 0.147 mol/dm^3, the suggested reactor volume is 1000 dm^3.

Data available:
At 300 K,
k_1 = 0.014 $(dm^3/mol)^{1/2}$ s^{-1}.
k_2 = 0.007 dm^3/(mol.s)
k_3 = 0.014 s^{-1}
k_4 = 0.45 dm^3/(mol.s)

(a) Plot the molar flow rates of each species along the volume (length) of the reactor on the same figure.
(b) 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.