The goal of the following exercises is to be able to describe the rates of transformation of chemical reactions and write the mole balances for different types of stirred-tank reactors.

Problem 1

The following liquid-phase reactions take place in a 150 L batch reactor operating in isothermal mode:

$A \rightarrow B + C$ avec $r_1 = k_1 \cdot C_A$

$2C + A \rightarrow 3D$ avec $r_2 = k_2 \cdot C_C^2 \cdot C_A$

$4C + 3D \rightarrow 3E$ avec $r_3 = k_3 \cdot C_C \cdot C_D$

The initial concentration of A is 3.2 mol/L, and the other chemical species are not present at the start of the reaction. The rate constant values k1, k2, and k3 are respectively $7.0 \cdot 10^{-3}$ (1/min), $3.0 \cdot 10^{-2}$ ($L^2/mol^2 \cdot min$), and $2.0 \cdot 10^{-4}$ (L/mol·min).

Determine the reaction time to achieve a conversion of 40 and 90% of species A and provide the final concentrations of A, B, C, D, and E.

Problem 2

The production of maleic anhydride by oxidation of benzene using vanadium peroxide as catalyst is described in the literature. The involved reactions are described below:

- $C_6H_6 + \frac{9}{2}O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O$

with $k_1 = 4280 \cdot \exp(-12660/T)$

- $C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$

with $k_2 = 70100 \cdot \exp\left(-\frac{15000}{T}\right)$

- $C_6H_6 + \frac{15}{2}O_2 \rightarrow 6CO_2 + 3H_2O$

with $k_3 = 26 \cdot \exp\left(-\frac{10800}{T}\right)$

These reactions are carried out in the presence of an excess of oxygen and behave as pseudo-first order reactions. At 848 K, the rate constants are: k1 = $1.4 \cdot 10^{-3}$ (1/s), $k_2 = 1.46 \cdot 10^{-3}$ (1/s), and $k_3 = 7.65 \cdot 10^{-5}$ (1/s). In this exercise, concentrations will be expressed in mol/kg-cat, and rates of reaction in mol/kg-cat/s.

These reactions are carried out in a batch reactor charged with a mass of catalyst of 230 kg (suspended in the stirred volume) and with an initial benzene concentration of 0.01 mol/m^3. What is the time needed to achieve a conversion of 85%?

Problem 3

A reactant A decomposes in three simultaneous reactions to form three products, only one of which is desired, B. These reactions are called Tambouze reactions:

$$A \xrightarrow{k_1} P \text{ with } r_1 = 0.0001 \frac{\text{mol}}{\text{L·s}}$$

$$A \xrightarrow{k_2} B \text{ with } r_2 = 0.0015 \cdot C_A \frac{\text{mol}}{\text{L·s}}$$

$$A \xrightarrow{k_3} Q \text{ with } r_3 = 0.008 \cdot C_A^2 \frac{\text{mol}}{\text{L·s}}$$

To carry out this transformation, we use a continuous stirred tank reactor (CSTR) of 1.564 m^3, followed in series by a plug flow reactor (PFR) of 0.6 m^3. The concentration of A at the inlet of the CSTR is 0.4 mol/L and the volumetric flow rate is 2 L/s.

(a) What is the time required to reach steady state in the first reactor?

(b) What is the conversion as well as the overall selectivity FB/FA at the outlet of the CSTR reactor?

Problem 4the

The second-order elementary liquid-phase reaction is carried out in a semi-batch reactor at 35°C.

$$C_6H_5COCH_2Br + C_6H_5N \rightarrow C_6H_5COCH_2NC_6H_5Br$$

The specific reaction rate constant is 0.0445 L/mol/min. The reactor is initially charged with 500 L of C_6H_5COCH_2Br at a concentration of 4 M. Then, 500 L of C_6H_5N at a concentration of 4 M are added at a constant rate of 10 L/min. At the same time, the reaction mixture is continuously pumped out of the reactor at a rate of 2 L/min.

What will be the conversion and the concentration of each species in the reactor after 10, 50, and 80 minutes, assuming that the tank is ideally mixed?