**Problem 4:** Consider the following liquid phase reactions occurring under adiabatic conditions, and in steady state. \( A \overset{k_1}{\rightarrow} B \), \( B \overset{k_2}{\rightarrow} 2C \) and \( A \overset{k_3}{\rightarrow} 2C \). The feed contains 20% A, 20% B, 20% C and 40% solvent (inert). Volumetric flow rate at the inlet is 0.1 m\(^3\)s\(^{-1}\) and the molar flow rate is 100 mol s\(^{-1}\).

The rate constants are given by \( k_1 = 10^3 e^{-\frac{4000}{T}} \) s\(^{-1}\), \( k_2 = 5 \times 10^4 e^{-\frac{4500}{T}} \) s\(^{-1}\) and \( k_3 = 10^4 e^{-\frac{3500}{T}} \) m\(^3\) mol\(^{-1}\) s\(^{-1}\). Inlet temperature is 350 K.

The specific heat capacities are independent of temperature and are given by \( C_{p-A} = C_{p-B} = 200 \) J/mol/K, \( C_{p-C} = 100 \) J/mol/K and \( C_{p-inert} = 150 \) J/mol/K. The heat of the reactions are \( \Delta H_1 = -80,000 \) J/mol A reacted, \( \Delta H_2 = +30,000 \) J/mol B reacted and \( \Delta H_3 = -50,000 \) J/mol A reacted and these are independent of temperature.

Determine the temperature and the concentrations of the species as a function of volume in a PFR (0 to 2 m\(^3\)).

If we use a CSTR instead, what would be the temperature and the concentrations of the species? Increment the size of CSTR from 1 to 2 m\(^3\) in steps of 0.1 m\(^3\).

**Solution:**

The design equations are

\[
\frac{dF_A}{dV} = r_A, \quad \frac{dF_B}{dV} = r_B \quad \text{and} \quad \frac{dF_C}{dV} = r_C.
\]

The rate equations are

\[
r_A = -(k_1C_A + k_3C_A^2), \quad r_B = (k_1C_A - k_2C_B) \quad \text{and} \quad r_C = 2(k_2C_B + k_3C_A^2)
\]

Liquid phase reaction, so the change in number of moles and the change in temperature will not affect the flow rate.

\[
C_A = \frac{F_A}{Q} \quad \text{and other species’ concentrations are written in a similar fashion.}
\]

The volumetric flow rate is 0.1 m\(^3\)s\(^{-1}\).

\( F_{T-in} = 100 \) mol/s

\( F_{A-in} = 20 \) mol/s

\( F_{B-in} = 20 \) mol/s

\( F_{C-in} = 20 \) mol/s

\( F_{I-in} = 40 \) mol/s

Heat balance (Energy balance):
Heat released due to reaction (in a small volume dV) = heat needed to raise the feed by the temperature dT

Let \( r_1 = (k_1 C_A) \), \( r_2 = (k_2 C_B) \) and \( r_3 = (k_3 C^2_A) \)

\[
\left[ (r_1)(-\Delta H_1) + (r_2)(-\Delta H_2) + (r_3)(-\Delta H_3) \right] dV = \sum_i (F_i \text{in} \ C_{p-i}) dT
\]

Therefore,

\[
\frac{dT}{dV} = \frac{\left[ (r_1)(-\Delta H_1) + (r_2)(-\Delta H_2) + (r_3)(-\Delta H_3) \right]}{\sum_i (F_i \text{in} \ C_{p-i})}
\]

\[
\frac{dT}{dV} = \frac{\left[ (k_1 C_A)(+80000) + (k_2 C_B)(-30000) + (k_3 C^2_A)(+50000) \right]}{(20 \times 200 + 20 \times 200 + 20 \times 100 + 40 \times 150)}
\]

\[
\frac{dT}{dV} = \frac{\left[ (k_1 C_A)(+80000) + (k_2 C_B)(-30000) + (k_3 C^2_A)(+50000) \right]}{16000}
\]

Pressure drop may or may not be negligible but it won’t affect the concentration or the rate of the reaction, so we will not worry about it here. It can be solved independently (if we are given the relevant properties).

We have to solve the heat and mass balance equations simultaneously.