Problem 1

For elementary reaction

A ⇄ B

the equilibrium conversion is 0.8 at 127°C and 0.5 at 227°C. Using the Van't Hoff equation, what is the heat of reaction?

Problem 2

The elementary, irreversible, organic liquid-phase reaction

A + B → C

is carried out adiabatically in a flow reactor. An equal molar feed in A and B enters at 27°C, and the volumetric flow rate is 2 L/s and C_{A0} = 0.1 kmol/m³.

Here is additional information about the reaction:

$H^{\circ}_{f\,A}(273\ K) = -20$ kcal/mol, $H^{\circ}_{f\,B}(273\ K) = -15$ kcal/mol, $H^{\circ}_{f\,C}(273\ K) = -41$ kcal/mol

$c_{p_A} = c_{p_B} = 15$ cal/mol/K and $c_{p_C} = 30$ cal/mol/K

$k = 0.01$ L/mol/s at 300 K and $E_a = 10$ kcal/mol

Let's first consider an adiabatic PFR reactor

1. Plot and then analyze the conversion and temperature as a function of PFR volume up to where X = 0.85. Describe the trends.
2. What is the maximum inlet temperature one could have so that the boiling point of the liquid (550 K) would not be exceeded even for complete conversion?
3. Plot and then analyze the conversion and temperature profiles up to a PFR reactor volume of 10 L for the case when the reaction is reversible with K_c = 10 m³/kmol at 450 K. Plot the equilibrium conversion profile. How are the trends different than part (**a**)?

Then, let's consider an adiabatic CSTR reactor

4. What is the CSTR volume necessary to achieve 90% conversion?

Batch reactor

5. The reaction is next carried out in a 25 dm^3 batch reactor charged with N_{A0} = 10 moles. Plot the number of moles of A, N_A, the conversion, and the temperature as a function of time.