All-in-one problem. Multiple reaction, change in molar flow rate, pressure drop, variable specific heat capacity, variable viscosity and cooling coils.

Gas phase reaction $A \rightarrow B$, $B \rightarrow 2C$ and $A \rightarrow 2C$ is conducted in a packed bed reactor. Feed contains 50% A, 25% B and 25% inert (all in mole %). MW of A = 60 g/mol, MW of inert = 28 g/mol. At the inlet, the pressure is $P_{in} = 10^6$ Pa (absolute). Assume ideal gas law. Total molar flow rate at the inlet is 20 gmol/s. The rate constants are given by $k_1 = 10^3 e^{-\frac{4000}{T}}$ s$^{-1}$, $k_2 = 10^4 e^{-\frac{5500}{T}}$ s$^{-1}$ and $k_3 = 50 e^{-\frac{3500}{T}}$ m$^3$ mol$^{-1}$ s$^{-1}$.

a. The heat of the reactions are $\Delta H_1 = -1,000$ J/mol A reacted, $\Delta H_2 = -12,000$ J/mol B reacted and $\Delta H_3 = -13,000$ J/mol A reacted, all at 300 K.

b. The specific heat capacities are functions of temperature. $C_{p-A} = C_{p-B} = 10 + 0.06 T + 6 \times 10^{-5} T^2$ J/mol/K, $C_{p-C} = 5 + 0.02 T + 2 \times 10^{-5} T^2$ J/mol/K and $C_{p-inert} = 15 + 0.05 T + 5 \times 10^{-5} T^2$ J/mol/K.

c. The viscosity is a function of temperature and is given by $\mu = 1.5 \times 10^{-6} \frac{T^{\frac{3}{2}}}{T+100}$ Pa-s.

d. There is a cooling coil with $U = 2 \times 10^2$ W m$^{-2}$K$^{-1}$, $A = 2$ m$^2$, and $T_C = 300$ K, cooling coil is wound evenly throughout the reactor. (i.e. cooling coil area per unit volume of reactor is a constant).

e. Use the Ergun equation

i. the bed contains particles of 3 mm dia, void fraction of 0.4, bed dia = 20 cm, bed length = 6 m, particle density = 5 g/cm$^3$.

ii. Note: Ergun equation is given by $f_p = \frac{\Delta p}{L} \frac{D_p}{\rho V_s^2} \left( \frac{\epsilon^3}{1-\epsilon} \right) = \frac{150}{Gr_p} + 1.75$

where $Gr_p = \frac{D_p V_s \rho}{(1-\epsilon) \mu}$

f. Determine the volumetric flow rate and the density of the feed at the inlet.

Solution:

The volumetric flow rate at the inlet is given by $Q_{in} = \frac{F_{in}}{P_{in}} = \frac{20 \times 8.314 \times 400}{10^6} = 0.066512$ m$^3$s$^{-1} = 66.512$ lit/s

$F_{A-in} = 10$ mol/s
$F_{B-in} = 5$ mol/s
$F_{C-in} = 0$ mol/s
$F_{I-in} = 5$ mol/s

Density of the feed at the inlet is given by $\rho_{in} = \frac{\text{mass flow rate at the inlet}}{\text{volumetric flow rate at the inlet}} = \frac{10 \times 60 + 5 \times 60 + 5 \times 28}{0.066512} = 15.636$ kg/m$^3$
Mass balance:

The design equations are
\[ \frac{dF_A}{dV} = r_A, \frac{dF_B}{dV} = r_B \text{ and } \frac{dF_C}{dV} = r_C. \]

The rate equations are
\[ r_A = -\left(k_1C_A + k_3C_A^2\right), \quad r_B = \left(k_1C_A - k_2C_B\right) \text{ and } r_C = 2\left(k_2C_B + k_3C_A^2\right) \]

Note that the $\Delta H$ values are also functions of temperature and concentration is a variable, that must be written in terms of other variables.

The volumetric flow rate will change because there is a change in temperature, pressure and in number of moles flowing per unit time.

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

Using ideal gas law, we can write
\[ Q = \frac{F_A RT}{P} = \frac{(F_A + F_B + F_C + F_I)RT}{P}, \text{ i.e. the volumetric flow rate can be written in terms of T, P and molar flow rates of each species.} \]

Therefore the concentration of each species at any location can be written as functions of T, P and molar flow rates of each species. We get the following equations
\[ \frac{dF_A}{dV} = \left( k_A F_A \frac{P}{(F_A + F_B + F_C + F_I)RT} + k_3 F_A^2 \left[ \frac{P}{(F_A + F_B + F_C + F_I)RT} \right]^2 \right) \] (1)
\[ \frac{dF_B}{dV} = \left( k_A F_A \frac{P}{(F_A + F_B + F_C + F_I)RT} - k_2 F_B \frac{P}{(F_A + F_B + F_C + F_I)RT} \right) \] (2)
\[ \frac{dF_C}{dV} = 2\left( k_2 F_B \frac{P}{(F_A + F_B + F_C + F_I)RT} + k_3 F_A^2 \left[ \frac{P}{(F_A + F_B + F_C + F_I)RT} \right]^2 \right) \] (3)

We should remember that the rate constants in the above equations are also functions of temperature.

Heat balance (Energy balance):

Heat released due to reaction (in a small volume $dV$) = heat needed to raise the feed by the temperature $dT$ + heat taken up by the cooling coils

Let $r_1 = (k_1C_A)$, $r_2 = (k_2C_B)$ and $r_3 = (k_3C_A^2)$
\[
\left[ (r_1)(-\Delta H_1) + (r_2)(-\Delta H_2) + (r_3)(-\Delta H_3) \right] dV = \sum_i \left( F_{in} C_{p,i} \right) dT + U \left( \frac{A}{V_{PFR}} \right) dV (T - T_c)
\]

Hence,

\[
\frac{dT}{dV} = \frac{\left[ (r_1)(-\Delta H_1) + (r_2)(-\Delta H_2) + (r_3)(-\Delta H_3) \right] - U \left( \frac{A}{V_{PFR}} \right) (T - T_c)}{\sum_i \left( F_{in} C_{p,i} \right)}
\]

But \( \Delta H \) here is a function of temperature. Therefore we need to write them separately. The specific heat capacities are functions of temperature. \( C_{p,A} = 10 + 0.06 T + 6 \times 10^{-5} T^2 \) J/mol/K, \( C_{p,C} = 5 + 0.02 T + 2 \times 10^{-5} T^2 \) J/mol/K and \( C_{p,inert} = 15 + 0.05 T + 5 \times 10^{-5} T^2 \) J/mol/K.

\[
\Delta H_{1p} = \Delta H_{1r} \left( T - T_{ref} \right) + \Delta C_p \left( T - T_{ref} \right) = \Delta H_{1r} \left( T - T_{ref} \right) + \left( C_{pB} - C_{PA} \right) \left( T - T_{ref} \right)
\]

\[
\Delta H_{2p} = \Delta H_{2r} \left( T - T_{ref} \right) + \Delta C_p \left( T - T_{ref} \right) = \Delta H_{2r} \left( T - T_{ref} \right) + \left( C_{pB} - 2C_{PC} \right) \left( T - T_{ref} \right)
\]

And likewise

\[
\Delta H_{3p} = \Delta H_{3r} \left( T - T_{ref} \right) + \Delta C_p \left( T - T_{ref} \right) = \Delta H_{3r} \left( T - T_{ref} \right) + \left( C_{pA} - 2C_{PC} \right) \left( T - T_{ref} \right)
\]

\[
\frac{dT}{dV} = \frac{\left[ (k_1 C_A)(\Delta H_1) + (k_2 C_B)(\Delta H_2) + (k_3 C_A^2)(\Delta H_3) \right] - U \left( \frac{A}{V_{PFR}} \right) (T - T_c)}{\left( F_A C_{pA} + F_B C_{pB} + F_C C_{pC} + F_I C_{pl} \right)} ---(4)
\]

Since the concentrations are written in terms of \( F_A, F_B, F_C, \) and \( F_I, \) along with \( P \) and \( T, \) we have the above equation in terms of dependent variables.

Pressure drop equation:

\[
\frac{dP_{new}}{dV} = -4 \pi D_c^2 \left( 150(1-\phi) \mu + 1.75 \right) \left( \frac{\rho V_s^2}{D_p} \right) \left( \frac{1-\phi}{\phi^5} \right) \frac{1}{10^5}
\]

Where \( P = P_{new} \times 10^5. \)

Here, \( \rho V_s = \left( \frac{\rho_{in} V_{in}}{A_{bed}} \right) = \left( \frac{\rho_{in}}{A_{bed}} \right) \left( \frac{4 \times Q_{in}}{\pi D_{bed}^3} \right) \)
Viscosity is a function of temperature $T$, 
$$\mu = 1.5 \times 10^{-6} \frac{T^{3/2}}{T+100}$$

Superficial velocity $V_s$ can be written in terms of volumetric flow rate $Q$, which can be written in terms of $T$, $P$ and molar flow rates of each species.

Therefore, the pressure can be written in terms of $T$, $P$ and molar flow rates of each species.

$$\frac{dp_{new}}{dV} = -\frac{4}{\pi D_c^2} \left( \frac{150(1-\phi)\mu}{D_p V_s \rho} + 1.75 \left( \frac{\rho V_s^2}{D_p} \right) \left( \frac{1-\phi}{\phi^2} \right) \frac{1}{10^5} \right) \tag{5}$$

The initial conditions are $T_{in} = 400$ K, $P_{in} = 10^6$ Pa, $F_{A-in} = 10$ mol/s, $F_{B-in} = 5$ mol/s, and $F_{C-in} = 0$ mol/s.

Numerically integrating the 5 equations with the above 5 conditions, we can get the answer.