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 $A \xrightarrow{k_1} B$, $B \xrightarrow{k_2} 2C$ and $A \xrightarrow{k_3} 2C$ is conducted in a packed bed reactor. Feed contains 50% A, 25% B and 25 % inerts (all in mole %). MW of A = 60 g/gmol, MW of inert = 28 g/gmol. 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}, $k_2 = 10^5 e^{-\frac{5500}{T}}$ s^{-1} and $k_3 = 50 e^{-\frac{3500}{T}}$ m^3 mol^{-1} s^{-1}.

   a. The heat of the reactions are ΔH_1 = -1,000 J/mol A reacted, ΔH_2 = -12,000 J/mol B reacted and ΔH_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
$$\mu = 1.5 \times 10^{-6} \frac{T^{\frac{3}{2}}}{T + 100} \text{ Pa-s..}$$
   d. There is a cooling coil with U = 2×10^2 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 $f_p = \frac{\Delta p}{L} \frac{D_p}{\rho V_s^2} \left(\frac{\varepsilon^3}{1-\varepsilon} \right) = \frac{150}{Gr_p} + 1.75$

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

   f. Determine the volumetric flow rate and the density of the feed at the inlet.
   g. Determine the molar flow rate and concentration profiles of A, B and C , and the pressure and temperature profiles in the reactor.

Solution:

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

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
$$\rho_{in} = \frac{\text{mass flow rate at the inlet}}{\text{volumetric flow rate at the inlet}} = \frac{10 \times 60 + 5 \times 60 + 5 \times 28}{0.066512} = 15.636 \frac{kg}{m^3}$$

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

$$r_A = -\left(k_1 C_A + k_3 C_A^2\right), \quad r_B = \left(k_1 C_A - k_2 C_B\right) \text{ and } r_C = 2\left(k_2 C_B + k_3 C_A^2\right)$$

Note that the ΔH 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 $Q = \dfrac{F_T RT}{P} = \dfrac{\left(F_A + F_B + F_C + F_I\right)RT}{P}$, 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

$$\frac{dF_A}{dV} = -\left(k_1 F_A \frac{P}{\left(F_A + F_B + F_C + F_I\right)RT} + k_3 F_A^2 \left[\frac{P}{\left(F_A + F_B + F_C + F_I\right)RT}\right]^2\right) \text{------------ (1)}$$

$$\frac{dF_B}{dV} = \left(k_1 F_A \frac{P}{\left(F_A + F_B + F_C + F_I\right)RT} - k_2 F_B \frac{P}{\left(F_A + F_B + F_C + F_I\right)RT}\right) \text{-------------(2)}$$

$$\frac{dF_C}{dV} = 2\left(k_2 F_B \frac{P}{\left(F_A + F_B + F_C + F_I\right)RT} + k_3 F_A^2 \left[\frac{P}{\left(F_A + F_B + F_C + F_I\right)RT}\right]^2\right) \text{---(3)}$$

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 $r_1 = \left(k_1 C_A\right)$, $r_2 = \left(k_2 C_B\right)$ and $r_3 = \left(k_3 C_A^2\right)$

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

Hence,

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

But ΔH here is a function of temperature. Therefore we need to write them separately. The specific heat capacities are functions of temperature. $C_{p\text{-}A} = C_{p\text{-}B} = 10 + 0.06\,T + 6\times10^{-5}\,T^2$ J/mol/K, $C_{p\text{-}C} = 5 + 0.02\,T + 2\times10^{-5}\,T^2$ J/mol/K and $C_{p\text{-}inert} = 15 + 0.05\,T + 5\times10^{-5}\,T^2$ J/mol/K.

$$\Delta H_1\big|_T = \Delta H_1\big|_{T_{ref}} + \Delta C_p\left(T-T_{ref}\right) = \Delta H_1\big|_{T_{ref}} + \left(C_{pB}-C_{PA}\right)\left(T-T_{ref}\right)$$

$$\Delta H_2\big|_T = \Delta H_2\big|_{T_{ref}} + \Delta C_p\left(T-T_{ref}\right) = \Delta H_2\big|_{T_{ref}} + \left(C_{pB}-2C_{PC}\right)\left(T-T_{ref}\right)$$

And likewise

$$\Delta H_3\big|_T = \Delta H_3\big|_{T_{ref}} + \Delta C_p\left(T-T_{ref}\right) = \Delta H_3\big|_{T_{ref}} + \left(C_{pA}-2C_{PC}\right)\left(T-T_{ref}\right)$$

$$\frac{dT}{dV}=\frac{\left[(k_1C_A)(\Delta H_1)+(k_2C_B)(\Delta H_2)+(k_3C_A^2)(\Delta H_3)\right]--U\left(\dfrac{A}{V_{PFR}}\right)\left(T-T_C\right)}{\left(F_AC_{pA}+F_BC_{pB}+F_CC_{pC}+F_IC_{pI}\right)} \qquad \text{---(4)}$$

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:

$$\frac{dp_{new}}{dV}=-\frac{4}{\pi D_c^2}\left(\frac{150(1-\phi)\mu}{D_pV_s\rho}+1.75\right)\left(\frac{\rho V_s^2}{D_p}\right)\left(\frac{1-\phi}{\phi^3}\right)\frac{1}{10^5}$$

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

Here, $\left(\rho V_s\right)=\left(\rho_{in}V_{s-in}\right)=\left(\rho_{in}\dfrac{Q_{in}}{A_{bed}}\right)=\left(\rho_{in}\dfrac{4\times Q_{in}}{\pi D_{bed}^2}\right)$

Viscosity is a function of temperature T, $\mu = 1.5 \times 10^{-6} \dfrac{T^{\frac{3}{2}}}{T+100}$

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.

$$\frac{dp_{new}}{dV} = -\frac{4}{\pi D_c^2} \left(\frac{150(1-\phi)\mu}{D_p V_s \rho} + 1.75 \right) \left(\frac{\rho V_s^2}{D_p} \right) \left(\frac{1-\phi}{\phi^3} \right) \frac{1}{10^5} \qquad \text{----(5)}$$

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

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

Molar flow rate vs Reactor Volume (m^3)

Temperature (K) vs Reactor Volume (m^3)

Presssure(atm) vs Reactor Volume (m^3)