Example 12-5 Parallel Reactions in a PFR with Heat Effects

The following gas-phase reactions occur in a PFR:

$$\text{Reaction 1:} \quad A \xrightarrow{k_1} B \qquad -r_{1A} = k_{1A}C_A \qquad \text{(E12-5.1)}$$

$$\text{Reaction 2:} \quad 2A \xrightarrow{k_2} C \qquad -r_{2A} = k_{2A}C_A^2 \qquad \text{(E12-5.2)}$$

Pure A is fed at a rate of 100 mol/s, a temperature of 150°C, and a concentration of 0.1 mol/dm^3. Determine the temperature and molar flow rate profiles down the reactor.

Additional information

$\Delta H_{Rx1A} = -20{,}000$ J/(mol of A reacted in reaction 1)

$\Delta H_{Rx2A} = -60{,}000$ J/(mol of A reacted in reaction 2)

$C_{P_A} = 90$ J/mol·°C

$C_{P_B} = 90$ J/mol·°C

$C_{P_C} = 180$ J/mol·°C

$Ua = 4000$ J/m^3·s·°C

$T_a = 100$°C (Constant)

$$k_{1A} = 10 \exp\left[\frac{E_1}{R}\left(\frac{1}{300} - \frac{1}{T}\right)\right] \text{s}^{-1}$$

$E_1/R = 4000$ K

$$k_{2A} = 0.09 \exp\left[\frac{E_2}{R}\left(\frac{1}{300} - \frac{1}{T}\right)\right] \frac{\text{dm}^3}{\text{mol}\cdot\text{s}}$$

$E_2/R = 9000$ K

Solution

The PFR energy balance becomes [cf. Equation (12-35)]

$$\frac{dT}{dV} = \frac{Ua(T_a - T) + (-r_{1A})(-\Delta H_{Rx1A}) + (-r_{2A})(-\Delta H_{Rx2A})}{F_A C_{P_A} + F_B C_{P_B} + F_C C_{P_C}} \quad \text{(E12-5.3)}$$

Mole balances:

$$\frac{dF_A}{dV} = r_A \quad \text{(E12-5.4)}$$

$$\frac{dF_B}{dV} = r_B \quad \text{(E12-5.5)}$$

$$\frac{dF_C}{dV} = r_C \quad \text{(E12-5.6)}$$

Rates:

Rate laws

$$r_{1A} = -k_{1A} C_A \quad \text{(E12-5.1)}$$

$$r_{2A} = -k_{2A} C_A^2 \quad \text{(E12-5.2)}$$

Relative rates

Reaction 1: $\frac{r_{1A}}{-1} = \frac{r_{1B}}{1}; \quad r_{1B} = -r_{1A} = k_{1A} C_A$

Reaction 2: $\frac{r_{2A}}{-2} = \frac{r_{2C}}{1}; \quad r_{2C} = -\frac{1}{2} r_{2A} = \frac{k_{2A}}{2} C_A^2$

Net rates:

$$r_A = r_{1A} + r_{2A} = -k_{1A} C_A - k_{2A} C_A^2 \quad \text{(E12-5.7)}$$

$$r_B = r_{1B} = k_{1A} C_A \quad \text{(E12-5.8)}$$

$$r_C = r_{2C} = \frac{1}{2} k_{2A} C_A^2 \quad \text{(E12-5.9)}$$

Stoichiometry (gas phase $\Delta P = 0$):

$$C_A = C_{T0}\left(\frac{F_A}{F_T}\right)\left(\frac{T_0}{T}\right) \quad \text{(E12-5.10)}$$

$$C_B = C_{T0}\left(\frac{F_B}{F_T}\right)\left(\frac{T_0}{T}\right) \quad \text{(E12-5.11)}$$

$$C_C = C_{T0}\left(\frac{F_C}{F_T}\right)\left(\frac{T_0}{T}\right) \quad \text{(E12-5.12)}$$

$$F_T = F_A + F_B + F_C \tag{E12-5.13}$$

$$k_{1A} = 10 \exp\left[4000\left(\frac{1}{300} - \frac{1}{T}\right)\right] \text{s}^{-1}$$

(T in K)

$$k_{2A} = 0.09 \exp\left[9000\left(\frac{1}{300} - \frac{1}{T}\right)\right] \frac{\text{dm}^3}{\text{mol} \cdot \text{s}}$$

Energy balance:

$$\frac{dT}{dV} = \frac{4000(373 - T) + (-r_{1A})(20{,}000) + (-r_{2A})(60{,}000)}{90F_A + 90F_B + 180F_C} \tag{E12-5.14}$$

The Polymath program and its graphical outputs are shown in Table E12-5.1 and Figures E12-5.1 and E12-5.2.

Note from Dr. Ford Versypt

Be cautious when following these example equations:

1. The program used here allows equations to be entered in any order. MATLAB and Python both require variables to be defined before they can be used.
2. The differential equations list and the explicit equations for k1a and k2a have parameter values plugged in. Instead you should leave the parameter names in the formulas and separately provide parameter values so that the values can be changed easily.

TABLE E12-5.1 POLYMATH PROGRAM

Differential equations
1 d(Fa)/d(V) = r1a+r2a
2 d(Fb)/d(V) = -r1a
3 d(Fc)/d(V) = -r2a/2
4 d(T)/d(V) = (4000*(373-T)+(-r1a)*20000+(-r2a)*60000)/(90*Fa+90*Fb+180*Fc)

Explicit equations
1 k1a = 10*exp(4000*(1/300-1/T))
2 k2a = 0.09*exp(9000*(1/300-1/T))
3 Cto = 0.1
4 Ft = Fa+Fb+Fc
5 To = 423
6 Ca = Cto*(Fa/Ft)*(To/T)
7 Cb = Cto*(Fb/Ft)*(To/T)
8 Cc = Cto*(Fc/Ft)*(To/T)
9 r1a = -k1a*Ca
10 r2a = -k2a*Ca^2

Calculated values of DEQ variables

	Variable	Initial value	Final value
1	Ca	0.1	2.069E-09
2	Cb	0	0.0415941
3	Cc	0	0.016986
4	Cto	0.1	0.1
5	Fa	100.	2.738E-06
6	Fb	0	55.04326
7	Fc	0	22.47837
8	Ft	100.	77.52163
9	k1a	482.8247	2.426E+04
10	k2a	553.0557	3.716E+06
11	r1a	-48.28247	-5.019E-05
12	r2a	-5.530557	-1.591E-11
13	T	423.	722.0882
14	To	423.	423.
15	V	0	1.

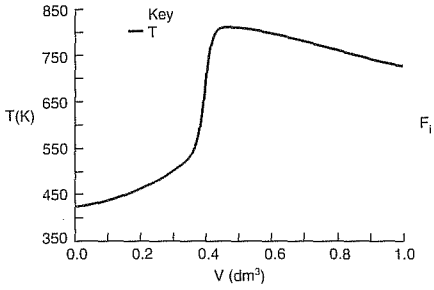

Figure E12-5.1 Temperature profile.

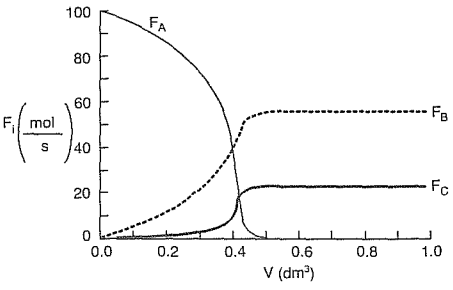

Figure E12-5.2 Profile of molar flow rates F_A, F_B, and F_C.