Josh Whitehead

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HW 5

1)a) $A \rightarrow 2P \qquad -r_A = k_1 C_A^2$

Assume:
- isothermal
- liquid

$1.5\dot{V}_{in} = \dot{V}_{out}$

Derive $\frac{dC_A}{dt}$ and $\frac{dC_P}{dt}$:

$$r_A V(t) = \frac{dN_A}{dt} = V\frac{dC_A}{dt} + C_A\frac{dV}{dt}$$

$$\dot{m} = \frac{dm}{dt} \rightarrow \rho \dot{V} = \frac{d\rho V}{dt} \rightarrow \frac{dV}{dt} = \dot{V} = (\dot{V}_{in} - \dot{V}_{out})$$

$$\therefore r_A V(t) = V\frac{dC_A}{dt} + C_A(\dot{V}_{in} - \dot{V}_{out})$$

$$\rightarrow \boxed{\frac{dC_A}{dt} = -C_A\left(k_1 C_A + \frac{(\dot{V}_{in} - \dot{V}_{out})}{V(t)}\right)}$$

$$\frac{dC_P}{dt} = r_P - \frac{(\dot{V}_{in} - \dot{V}_{out})C_P}{V(t)} \longrightarrow r_P = -2r_A$$

$$\therefore \boxed{\frac{dC_P}{dt} = -2k_1 C_A^2 - \frac{(\dot{V}_{in} - \dot{V}_{out})C_P}{V(t)}}$$

where $V(t) = V_0 + t(\dot{V}_{in} - \dot{V}_{out})$

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1) b) Find n_p leaving reactor @ 2 hours:

$\dot{V}_{in} = 10 \frac{L}{hr}$

$t = 2\ hr$

$V_0 = 1000$

$n^0_{A_0} = 200$

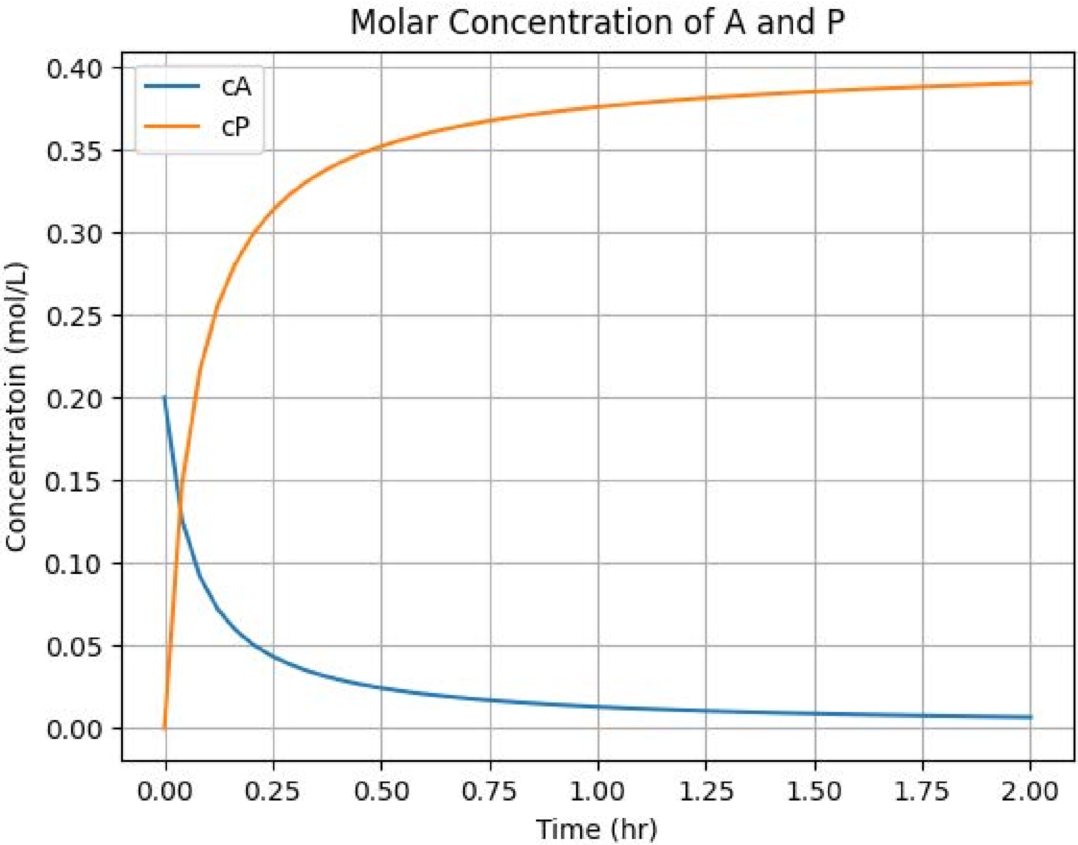
$k_1 = 0.02 \frac{L}{mol \cdot sec}$

$C_{A_0} = \frac{n_{A_0}}{V_0} = 0.2 \frac{mol}{L}$

- used python to solve ODE's in part A

C_p @ 2hrs $= 0.39 \frac{mol}{L}$

$n_p = C_p \cdot \dot{V}_{out} \cdot 2\ hours = 0.39 \cdot 15 \cdot 2 = \boxed{11.7\ mol}$



Molar Concentration of A and P
cA
cP
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Concentratoin (mol/L)
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
2.00
Time (hr)

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2)a) $\dot{v}(z) = \dot{v}_0 \left(1 - \frac{z}{L}\right)$ $A \rightarrow P$

assume:
- isobaric
- isothermal

Determine $F_{A leak}(z)$:

$\frac{d\dot{v}_0}{dz} \Rightarrow \dot{v}_{leak}$ $\therefore$ $\boxed{F_{A leak}(z) = \frac{d\dot{v}}{dz} \cdot C_A \cdot \Delta z}$

2)b) $F_{in} = F_{out} + F_{leak}$

$F = \frac{dN}{dt} = rV \rightarrow F_{in} = r_A A_c z = -k C_A A_c z$

$F_{out} = -k C_A A_c \Delta z$

$\therefore -k \cancel{C_A} A_c z = -k \cancel{C_A} A_c \Delta z + \frac{d\dot{v}}{dz} \cancel{C_A} \Delta z$

$\rightarrow \boxed{k A_c z = k A_c \Delta z - \frac{d\dot{v}}{dz} \Delta z}$

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2)c) $\Delta z = 0$

$\rightarrow \cancel{F_{in} = kA_c z C_A = F_{A} v_{in} C_{A0}(1-X_A)}$

$$\frac{dF_A}{dV} = -r_A = \frac{d(v C_A)}{A_c dz} = kC_A$$

$$\rightarrow kC_A A_c = v\frac{dC_A}{dz} + C_A\frac{dv}{dz}$$

$$kC_A A_c = v C_{A0}\frac{d(1-X_A)}{dz} + C_A\frac{dv}{dz}$$

$$\rightarrow kC_A A_c = v C_{A0}\left[\cancel{\frac{d}{dz}(1)} - \frac{dX_A}{dz}\right] + C_A\frac{dv}{dz}$$

$$\therefore \boxed{kC_A A_c = v C_{A0}\left(-\frac{dX_A}{dz}\right) + C_A\frac{dv}{dz}}$$

$\cancel{C_{A0} = \frac{F_{A0}}{v_0}} \quad \cancel{F_{A0} = v C_{A0}}$

$$C_{A0} = \frac{F_{A0}}{v_0}$$

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2)d) $k C_A A_c = -v C_{A_0} \frac{dx_A}{dz} + C_A \frac{dv}{dz}$

$$\rightarrow \frac{dx_A}{dz} = \frac{C_A \left(kA_c - \frac{dv}{dz}\right) v_0}{-v \, \cancel{C_{A_0}} \, F_{A_0}}$$

$$v(z) = v_0\left(1-\frac{z}{L}\right) \rightarrow \frac{dv}{dz} = \frac{-1}{L}$$

$$\therefore \boxed{\frac{dx_A}{dz} = \frac{-C_A\left(kA_c + \frac{1}{L}\right)\cancel{v_0}}{F_{A_0}\cancel{v_0}\left(1-\frac{z}{L}\right)}}$$

$$= \frac{-C_A\left(k A_c + \frac{1}{L}\right)}{F_{A_0} - \frac{F_{A_0} z}{L}} = \cancel{-C_A(kA} \quad \frac{-C_A k A_c - \frac{C_A}{L}}{F_{A_0} - \frac{F_{A_0} z}{L}}$$

$$= \frac{-L C_A A_c k - C_A}{\cancel{L}} \cdot \frac{\cancel{L}}{F_{A_0} L - F_{A_0} z}$$

$$\cancel{dx} \boxed{= -\frac{C_A(L A_c k - 1)}{F_{A_0}(L-z)}}$$

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2) e) $$\frac{dx_A}{dz} = \frac{-C_A(LA_c k - 1)}{F_{A0}(L-z)}$$

$$\rightarrow x_A = \frac{-C_A(LA_c k - 1)}{F_{A0}} \int_0^z \frac{1}{(L-z)} dz$$

$$\rightarrow \boxed{x_A = \frac{+C_A(LA_c k - 1)}{F_{A0}} \ln(L-z)}$$