

① a)  $r_{Br} = r_{Br1} + r_{Br2} + r_{Br3}$

$$r_1 = \frac{r_{Br1}}{2} = \frac{r_{Br2}}{2} \rightarrow r_{Br1} = 2k_1 [Br_2] - 2k_{-1} [Br]^2$$

$$r_{Br} = 2k_1 [Br_2] - 2k_{-1} [Br]^2 - k_2 [Br][H_2] + k_{-2} [H][HBr] + k_3 [H][Br_2] \quad \textcircled{I}$$

$$r_H = r_{H1} + r_{H2} + r_{H3}$$

$$= k_2 [Br][H_2] - k_{-2} [H][HBr] - k_3 [H][Br_2] \quad \textcircled{II}$$

b)  $r_{HBr} = k_2 [Br][H_2] - k_{-2} [H][HBr] + k_3 [H][Br_2] \quad \textcircled{III}$

To get  $[Br]$  use the fact that step 1 is always QE:

$$r_1 = 0 = k_1 [Br_2] - k_{-1} [Br]^2$$

$$\downarrow$$

$$[Br] = \sqrt{\frac{k_1}{k_{-1}}} [Br_2]^{1/2} \quad \textcircled{IV}$$

To get  $[H]$  for the general case, apply PSSH to  $\textcircled{II}$ :

$$r_H = 0 = k_3 [H][Br_2] - k_{-2} [H][HBr] + k_2 [Br][H_2]$$

$$\downarrow$$

$$[H] = \frac{k_2 [Br][H_2]}{k_3 [Br_2] + k_{-2} [HBr]} \quad \textcircled{V}$$

Combine (III), (IV), and (V):

$$r_{\text{HBr}} = \frac{k_2 \sqrt{\frac{k_1}{k_{-1}}} [\text{Br}_2]^{1/2} [\text{H}_2] - \frac{k_{-2} k_2 \sqrt{\frac{k_1}{k_{-1}}} [\text{Br}_2]^{1/2} [\text{H}_2] [\text{HBr}]}{k_3 [\text{Br}_2] + k_{-2} [\text{HBr}]} + \frac{k_3 [\text{Br}_2]^{3/2} k_2 \sqrt{\frac{k_1}{k_{-1}}} [\text{H}_2]}{k_3 [\text{Br}_2] + k_{-2} [\text{HBr}]}$$

← most common form

↓ algebra

$$r_{\text{HBr}} = \frac{2 k_2 k_3 \sqrt{\frac{k_1}{k_{-1}}} [\text{Br}_2]^{3/2} [\text{H}_2]}{k_3 [\text{Br}_2] + k_{-2} [\text{HBr}]}$$

← prettiest form

c)

$$r_{\text{HBr}} = \frac{2 k_2 k_3 \sqrt{\frac{k_1}{k_{-1}}} [\text{Br}_2]^{3/2} [\text{H}_2]}{k_3 [\text{Br}_2] + k_{-2} [\text{HBr}]}$$

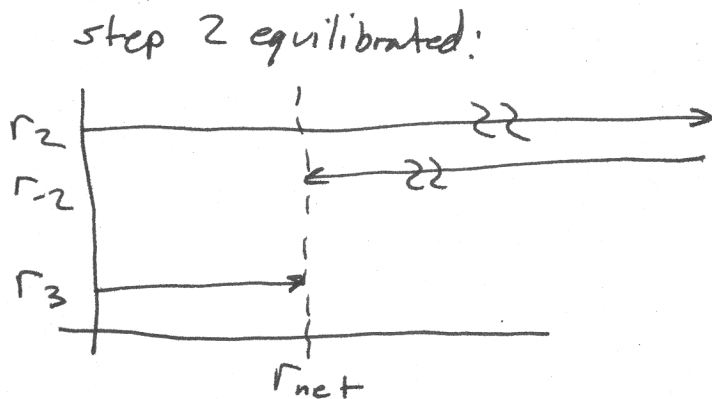
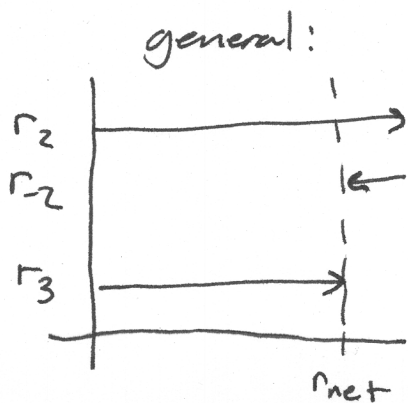
↓ step 2 equilibrated

$$= \left[ 2 \frac{k_2}{k_{-2}} k_3 \sqrt{\frac{k_1}{k_{-1}}} \frac{[\text{Br}_2]^{3/2} [\text{H}_2]}{[\text{HBr}]} \right]$$

K<sub>2</sub> ←

This happens if  $k_{-2} \gg k_3$

d)



$$e) \text{ PFR: } \frac{dF_{\text{Br}_2}}{dV} = r_{\text{Br}_2}$$

$$\begin{aligned} &\longrightarrow F_{\text{Br}_2} = F_{\text{Br}_2 0} (1-X) \longrightarrow dF_{\text{Br}_2} = -F_{\text{Br}_2 0} dX \\ -F_{\text{Br}_2 0} \frac{dX}{dV} &= r_{\text{Br}_2} = -k' C_{\text{Br}_2}^{3/2} \end{aligned}$$

↳ liquid phase:

$$F_{\text{Br}_2 0} \frac{dX}{dV} = k' C_{\text{Br}_2 0}^{3/2} (1-X)^{3/2} \quad C_{\text{Br}_2} = C_{\text{Br}_2 0} (1-X)$$

$$\int_0^{X_F} \frac{dX}{(1-X)^{3/2}} = \frac{k' C_{\text{Br}_2 0}^{3/2}}{F_{\text{Br}_2 0}} \int_0^V dV$$

$$V = \frac{2 F_{\text{Br}_2 0}}{k' C_{\text{Br}_2 0}^{3/2}} \left[ (1-X)^{-1/2} \right]_0^{0.7} = \boxed{2.05 \text{ L}}$$

$$F_{\text{Br}_2 0} = 12 \frac{\text{mol}}{\text{min}}$$

$$k' = 4.3 \frac{\text{L}^{1/2}}{\text{mol}^{1/2} \text{min}}$$

$$C_{\text{Br}_2 0} = \frac{12 \frac{\text{mol}}{\text{min}}}{7 \frac{\text{L}}{\text{min}}} = \frac{12}{7} \frac{\text{mol}}{\text{L}}$$

2.

(a) In - Out + R<sub>rxn</sub> = Accumulation

$$V_0 C_{max} - V_0 C_A + 0 = V \frac{dC_A}{dt} + C_A \left( \frac{dV}{dt} \right) \rightarrow 0 \quad \text{liquid phase}$$

$$V_0 (C_{max} - C_A) = -V \frac{d(C_{max} - C_A)}{dt}$$

$$\frac{d(C_{max} - C_A)}{C_{max} - C_A} = -\frac{V_0}{V} dt$$

$$\ln(C_{max} - C_A) \Big|_0^{C_A} = -\frac{V_0}{V} t$$

$$\frac{C_{max} - C_A}{C_{max}} = e^{-\frac{V_0}{V} t}$$

$$C_A = C_{max} \left( 1 - e^{-\frac{V_0}{V} t} \right) \quad (t \geq 0)$$

(b) 0<sup>th</sup> order rxn  $\bar{V}_A = -k$

In - Out + R<sub>rxn</sub> = Accumulation

$$V_0 C_{max} - V_0 C'_A - kV = V \frac{dC'_A}{dt} + C'_A \left( \frac{dV}{dt} \right) \rightarrow 0$$

$$V_0 \left( C_{max} - C'_A - \frac{kV}{V_0} \right) = -V \frac{d \left( C_{max} - C'_A - \frac{k}{V_0} \right)}{dt}$$

$$\ln \frac{C_{max} - C'_A - \frac{kV}{V_0}}{C_{max} - \frac{k}{V_0}} = -\frac{V_0}{V} t$$

$$C'_A = \left( C_{max} - \frac{kV}{V_0} \right) \left( 1 - e^{-\frac{V_0}{V} t} \right)$$

(c)

① Without rxn, steady state CSTR

$$V_0 C_{max} - V_0 C_{A,ss} = 0 \quad C_{A,ss} = C_{max}$$

to reach 99% of  $C_{A,ss}$ , then ~~is~~ by looking at the results from part (a)

$$C_A = C_{max} (1 - e^{-\frac{V_0}{V} t_1}) \Rightarrow t_1 = \frac{2V}{V_0} \ln 10$$
$$C_A = 0.99 C_{max}$$

② With 0th order rxn, steady state CSTR

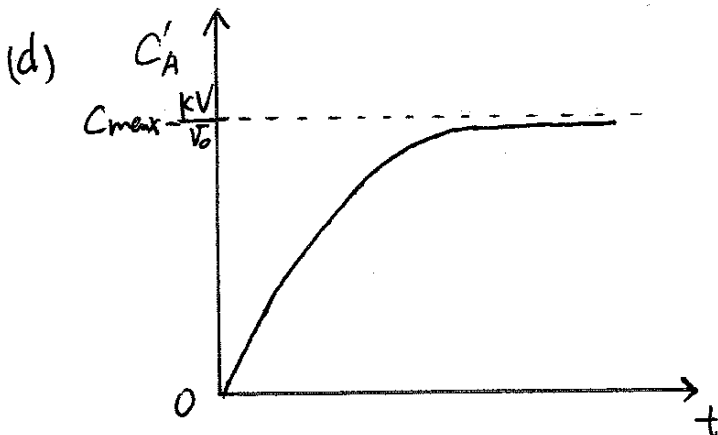
$$V_0 C_{max} - V_0 C'_{A,ss} - kV = 0$$

$$C'_{A,ss} = \frac{-kV + V_0 C_{max}}{V_0} = C_{max} - \frac{kV}{V_0}$$

To reach 99% of  $C'_{A,ss}$ , by looking at the results from part (b)

$$C'_A = (C_{max} - \frac{kV}{V_0}) (1 - e^{-\frac{V_0}{V} t_2}) \Rightarrow t_2 = \frac{2V}{V_0} \ln 10$$
$$C'_A = 0.99 (C_{max} - \frac{kV}{V_0})$$

The reaction doesn't change the time



### 3.a) Stoichiometric Table

Species	In	<del>Out</del> Change	Out before condensation	Out after condensation
A	$F_{A0}$	$-F_{A0} X_A$	$F_{A0}(1-X_A)$	$F_{A0}(1-X_A)$
B	0	$\frac{1}{2} F_{A0} X_A$	$\frac{1}{2} F_{A0} X_A$	$y_B F_T'$
C	0	$\frac{1}{2} F_{A0} X_A$	$\frac{1}{2} F_{A0} X_A$	$\frac{1}{2} F_{A0} X_A$
I	$F_{I0} = F_{A0}$	0	$F_{I0} = F_{A0}$	$F_{I0} = F_{A0}$
			$F_T = 2F_{A0}$	$F_T' = F_{A0} \left(2 - \frac{1}{2} X_A\right) + y_B F_T'$
				$\Rightarrow F_T' = \frac{F_{A0} \left(2 - \frac{1}{2} X_A\right)}{1 - y_B}$

b) Condensation begins when  $F_T = F_T'$

$$2F_{A0} = \frac{F_{A0} \left(2 - \frac{1}{2} X_A\right)}{1 - y_B} \rightarrow 0.2$$

$$\Rightarrow 1.6 = 2 - 0.5 X_A$$

$$\Rightarrow \boxed{X_A = 0.8}$$

c) Before condensation:  $2A(g) \rightarrow B(g) + C(g)$

$$S=0, \epsilon=0$$

$$r_A = -2k C_A^2, \quad C_A = \frac{C_{A0} (1 - X_A)}{1 + \epsilon X_A}$$

$$r_A = -2 C_{A0}^2 (1 - X_A)^2$$

$$C_{A0} = \frac{F_{\text{total},0} \times y_{A0}}{v} = \frac{10 \times 0.5 \text{ mol/litre}}{1} = 5 \text{ mol/litre}$$

$$\therefore \boxed{r_A = -50 (1 - X_A)^2} \text{ (mol/litre-min)}$$

After condensation,

$$C_A = \frac{F_A}{V}$$

$$V = v_0 \frac{F_T'}{F_{Total,0}} = v_0 \times \frac{F_{A0} (2 - \frac{1}{2} X_A)}{(1 - y_B)} = \frac{v_0 (1 - \frac{1}{4} X_A)}{(1 - y_B)}$$

$$C_A = \frac{F_{A0} (1 - X_A) (1 - y_B)}{v_0 (1 - \frac{1}{4} X_A)} = \frac{C_{A0} (1 - X_A) (1 - y_B)^{0.2}}{(1 - \frac{1}{4} X_A)}$$

$$\therefore C_A = 4 \frac{(1 - X_A)}{(1 - \frac{1}{4} X_A)} \text{ mol/litre}$$

$$\therefore r_A = -2k C_A^2$$

$$r_A = -32 \frac{(1 - X_A)^2}{(1 - \frac{1}{4} X_A)^2} \text{ (mol/litre-min)}$$

d)  $X_A = 0.95$ , condensation of B

$$V = \frac{F_{A0} X_A}{-r_A|_{\text{exit}}} = \frac{5 \times 0.95}{32 \frac{(1 - 0.95)^2}{(1 - \frac{1}{4} \times 0.95)^2}} \text{ litre}$$

$$= 34.5 \text{ litre}$$

e)  $F_A = 5(1 - 0.95) \text{ mol/min} = 0.25 \text{ mol/min}$

$$F_B' = \frac{5(2 - 0.5 \times 0.95)}{1 - 0.2} = 9.53125 \text{ mol/min}, F_B = y_B F_T' = 1.90625 \text{ mol/min}$$

$$F_C = \frac{1}{2} \times 5 \times 0.95 = 2.375 \text{ mol/min}, F_I = 5 \text{ mol/min}$$

mole fraction  $y_i = F_i / F_T'$

$$y_A = 0.026, F_B = 0.2, F_C = 0.249, F_I = 0.524$$

4. a)

Total material balance.

$$\text{Accumulation} = \text{In} - \text{Out} + \text{Generation}$$

$$\frac{d(V\rho)}{dt} = -v\rho \Rightarrow \boxed{\frac{dV}{dt} = -v} \quad (1)$$

$\rho$  constant,  $V = A_c z$ .

$$A_c \frac{dz}{dt} = -a\sqrt{2gz}$$

$$\frac{dz}{\sqrt{z}} = \alpha dt, \quad \alpha = -\frac{a\sqrt{2g}}{A_c}, \quad \alpha < 0.$$

at  $t=0, z = z_0$ .

$$2(\sqrt{z} - \sqrt{z_0}) = \alpha t.$$

$$z = \left(\sqrt{z_0} + \frac{\alpha t}{2}\right)^2.$$

$$\boxed{V = A_c z = A_c \left(\sqrt{z_0} + \frac{\alpha t}{2}\right)^2} \quad (2)$$

where  $\beta = \frac{\alpha}{2} = -\frac{a}{A_c} \sqrt{\frac{g}{2}}$ .

b) General mole balance

$$\text{In} - \text{Out} + \text{Gen} = \text{Acc.}$$

$$-C_A v + r_A V = \frac{d(N_A)}{dt}$$

$$-C_A v - k C_A V = \frac{d(C_A V)}{dt} = V \frac{dC_A}{dt} + C_A \frac{dV}{dt}$$

$$\Rightarrow -C_A v - k C_A V = V \frac{dC_A}{dt} - C_A v \quad \left[ \frac{dV}{dt} = -v \text{ from } \textcircled{1} \right]$$



$$\Rightarrow \boxed{\frac{dC_A}{dt} = -kC_A}$$

c) at  $t=0$ ,  $C_A = C_{A0}$  Integrating,

$$\therefore \boxed{C_A = C_{A0} e^{-kt}}$$

Same as for a batch reactor, uniformly

We are taking out the contents, without any selectivity, for any particular reactant and conc<sup>n</sup> is independent of the volume of liquid in the reactor, because it is uniformly mixed reactor.

$$\begin{aligned} d) N_A(t) &= C_A(t) \cdot V(t) \\ &= C_{A0} e^{-kt} \cdot A_c \cdot (\sqrt{z_0} + \beta t)^2 \end{aligned}$$

$$e) \frac{N_B|_{\text{leak}}}{N_B|_{\text{without leak}}} = \frac{(C_{A0} - C_A) \cdot V(t)}{(C_{A0} - C_A) \cdot V_0} \quad [C_B = C_{A0} - C_A]$$

$$\begin{aligned} &= \frac{A_c \cdot z}{A_c \cdot z_0} = \frac{z}{z_0} \\ &= \frac{(\sqrt{z_0} + \frac{\alpha t}{2})^2}{z_0} \end{aligned}$$