PRACTICAL SESSION 1

EX. 1

CONSTANT VOLUME BATCH REACTOR

$\rho = const \qquad A \longrightarrow B \qquad K = 0.01 \ s^{-1}$

$c_A^\circ = 2 \ \frac{mol}{\ell}$
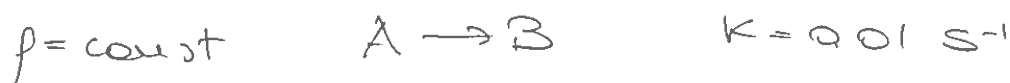
$r = K c_A \begin{cases} R_A = -K c_A \\ R_B = K c_A \end{cases} \qquad \begin{cases} \dfrac{dc_A}{dt} = -K c_A \\ \dfrac{dc_B}{dt} = K c_A \end{cases}$

$\dfrac{dc_A}{dt} = -K c_A \qquad \Rightarrow \qquad -c_A^\circ \dfrac{dx}{dt} = -K c_A^\circ (1-x)$

$\begin{cases} \dfrac{dx}{dt} = K(1-x) \\ x(t=0) = 0 \end{cases} \qquad \longrightarrow \qquad \dfrac{dx}{x-1} = -K \, dt$

$\qquad\qquad\qquad\qquad\qquad\qquad ln \dfrac{x-1}{(x-1)_0} = -Kt$

$\qquad\qquad\qquad\qquad\qquad\qquad \dfrac{x-1}{-1} = -Kt$

$$\boxed{x = 1 - \exp(-Kt)}$$

$x(\tau) = 1 - \exp(-K\tau)$

$$\boxed{\tau = -\dfrac{1}{K} \, ln(1-x)}$$

$\qquad\qquad\qquad\qquad\qquad \tau(x=90\%) = 230 \ s$

$\qquad\qquad\qquad\qquad\qquad \tau(x=99.9\%) = 691 \ s$

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EX 2.

CONSTDNT VOLUME BATCH REACTOR

$$A \longrightarrow B \qquad \tau = k\, c_A^\mu \;,\; \mu \neq 1$$
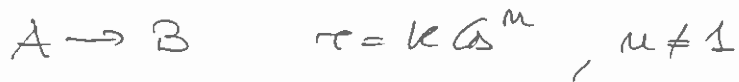
$$\frac{dc_A}{dt} = -k\, c_A^\mu \quad \Rightarrow \quad -c_A^0 \frac{dX}{dt} = -k\, c_{A0}^\mu (1-X)^\mu$$

$$\left|\begin{array}{l} \dfrac{dX}{dt} = k\, c_{A0}^{\mu-1}(1-X)^\mu \\[2mm] X(t=0) = 0 \end{array}\right. \qquad\qquad (1-X)^{-\mu}\, dX = k\, c_{A0}^{\mu-1}\, dt$$

$$\int (1-X)^{-\mu}\, dX = k\, c_{A0}^{\mu-1}\, t$$

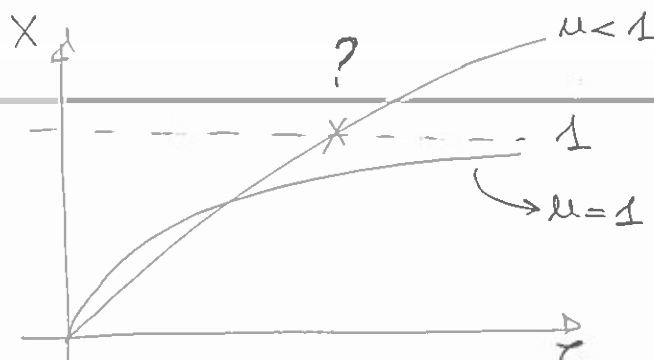$$\int (1-X)^{-\mu}\, dX = \;\ldots\; = -\int y^{-\mu}\, dy = -\left[\frac{y^{-\mu+1}}{-\mu+1}\right]$$

$$y \overset{\text{def}}{=} 1 - X$$

$$-\left[\frac{(1-X)^{-\mu+1}}{-\mu+1}\right]_0^X = k\, c_{A0}^{\mu-1}\, t$$

$$-\left[\frac{(1-X)^{-\mu+1} - 1}{-\mu+1}\right] = \frac{(1-X)^{-\mu+1} - 1}{\mu-1} = k\, c_{A0}^{\mu-1}\, t$$

$$\tau(X) = \frac{(1-X)^{-\mu+1} - 1}{k\, c_{A0}^{\mu-1}(\mu-1)} \qquad\qquad \left|\begin{array}{ll} \mu = \tfrac{1}{2} & \tau(90\%) = 1935\ s \\[3mm] \mu = 2 & \tau(90\%) = 950\ s \end{array}\right.$$

EX. 3

CSTR at constant density

$$A + B \rightarrow C \qquad c = k c_A c_B$$

$$k = 0.05 \frac{\ell}{mol\, s}$$

$$c_{A0} = 3 \frac{mol}{\ell}$$

$$c_{B0} = 4 \frac{mol}{\ell}$$

$$F_A^° - F_A + R_A V = 0 \qquad \Rightarrow \qquad Q(c_{A0} - c_A) + R_A V = 0$$

$$Q(c_{A0} - c_{A0}(1-x)) - k\, c_{A0}(1-x)\, c_{A0}(\vartheta_B^° - x)\, V = 0$$

$$Q c_{A0} x - k c_{A0}^2 (1-x)(\vartheta_B^° - x)\, V = 0 \qquad \tau \stackrel{def}{=} \frac{V}{Q}$$

$$x - k c_{A0}(1-x)(\vartheta_B^° - x)\, \tau = 0 \qquad \vartheta_B^° = \frac{c_B^°}{c_A^°}$$

$$\tau = \frac{x}{k c_{A0}(1-x)(\vartheta_B^° - x)} = \dots = \frac{x}{k(1-x)(c_B^° - c_{A0} x)}$$

$$\tau(95\%) = 330\, s$$

Observation

$$C_B = c_{B0} - c_{A0} x$$
$$C_A = c_{A0} - c_{A0} x$$

$$C_B - C_A = c_{B0} - c_{A0} \stackrel{def}{=} \Delta c_0 = const$$

$$C_B = c_A + \Delta c_0$$

$$c_B^° = c_A^° + \Delta c_0 \qquad \Rightarrow \qquad c_B^° - x c_A^° = \dots = c_A^°(1-x) + \Delta c_0$$

$$\tau = \frac{x}{k(1-x)(c_A^°(1-x) + \Delta c_0)}$$

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EX. 4

CONSTANT DENSITY CSTR

$$A \rightleftharpoons B \qquad r = K_f C_A - K_b C_B$$

$$\begin{cases} C_A^\circ = 1 \text{ mol}/\ell \\ C_B^\circ = 0 \end{cases}$$

$$\begin{cases} K_f = 0.5 \text{ min}^{-1} \\ K_b = 0.1 \text{ min}^{-1} \end{cases}$$
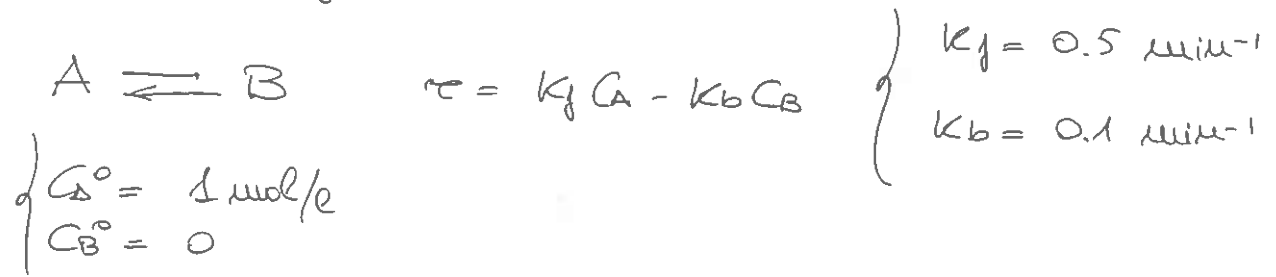
Equilibrium

$$K_f C_{Aeq} = K_b C_{Beq}$$

$$K_f C_{A0}(1 - X_{eq}) = K_b C_{A0} X_{eq}$$

$$X_{eq} = \frac{K_f}{K_f + K_b} \qquad X_{eq} = 5/6 > 50\% \quad \checkmark$$

Residence time

$$\dot{Q}(C_A^\circ - C_A) + R_A V = 0$$

$$\dot{Q} C_{A0} X - (K_f C_A - K_b C_B) V = 0$$

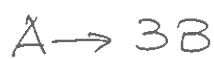$$C_{A0} X - (K_f C_{A0}(1-X) - K_b C_A^\circ X) \tau = 0$$

$$X - (K_f(1-X) - K_b X) \tau = 0$$

$$\boxed{\tau = \frac{X}{K_f(1-X) - K_b X}} \qquad \tau(50\%) = 2.5 \text{ min}$$

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EX. 5

CSTR with non constant density

$$A \rightarrow 3B \qquad r = K C_A^2 \qquad K = 0.5 \frac{\ell}{min \cdot mol}$$

$$
\left\{
\begin{array}{l}
C_A^\circ = 3 \frac{mol}{\ell} \\
C_B^\circ = 0 \\
F_A^\circ = 0.2 \frac{mol}{s}
\end{array}
\right.
$$

$$\dot{F}_A^\circ - \dot{F}_A + R_A V = 0$$

$$C_A = C_{A0} \frac{1-X}{1+2X}$$

$$\dot{Q} = \dot{Q}_0 (1 + \varepsilon X)/\gamma^*$$
$$= \dot{Q}_0 (1 + 2X)$$

$$C_j = C_{A0} \frac{\Theta_j^\circ + \nu_j X}{1 + \varepsilon X} \gamma^*$$

$$\gamma^* = \frac{T^\circ P}{T P_0} = \dots = 1$$

$$\varepsilon = \frac{F_A^\circ}{F_{tot}^\circ} \delta = 1 \cdot (3-1) = 2$$

$$\dot{Q}_0 C_{A0} - \dot{Q} C_A - K C_A^2 V = 0$$

$$\dot{Q}_0 C_{A0} - \dot{Q}_0 (1+2X) C_{A0} \frac{1-X}{1+2X} - K C_{A0}^2 \frac{(1-X)^2}{(1+2X)^2} V = 0$$

$$\dot{Q}_0 C_{A0} - \dot{Q}_0 C_{A0} (1-X) - K C_{A0} \cdot C_{A0} \frac{(1-X)^2}{(1+2X)^2} \cdot V = 0$$

$$1 - (1-X) - K C_{A0} \frac{(1-X)^2}{(1+2X)^2} \cdot \tau = 0$$
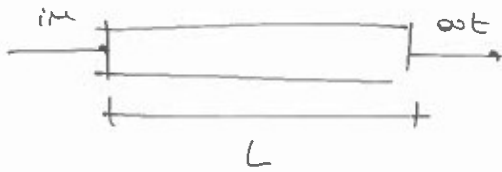
$$X - K C_{A0} \frac{(1-X)^2}{(1+2X)^2} \tau = 0$$

$$\boxed{\tau = \frac{X (1+2X)^2}{K C_{A0} (1-X)^2}} \qquad\qquad X = \frac{\dot{F}_A^\circ}{K C_{A0}^2} \frac{(1+2X)^2}{(1-X)^2}$$

$$\tau (95\%) = 734.7 \ min$$

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REACTIONS IN SERIES IN A PFR (constant density)

$L = 100\ m$

$d = 0.08\ m$

$T = 750°C$

$P = 3\ bar$

$\dot{F}_A^° = 20\ \frac{kmol}{h}$

$\dot{F}_B^° = \dot{F}_C^° = 0$

$$A \xrightarrow{K_1} B \xrightarrow{K_2} C$$

$$\begin{cases} r_1 = K_1 C_A \\ r_2 = K_2 C_B \end{cases}$$

$$\dot{Q} = \frac{\dot{F}_A^° \cdot MW_A}{\rho}$$

$$\begin{cases} \dfrac{dC_A}{dt} = -K_1 C_A \\[2mm] \dfrac{dC_B}{dt} = K_1 C_A - K_2 C_B \\[2mm] \dfrac{dC_C}{dt} = K_2 C_B \end{cases} + \quad ICs \begin{cases} C_A(0) = C_A^° = \dot{F}_A^°/\dot{Q} \\[2mm] C_B(0) = C_B^° = 0 \\[2mm] C_C(0) = C_C^° = 0 \end{cases}$$

$$\frac{dC_A}{dt} = -K_1 C_A \quad \Rightarrow \quad C_A = C_{A0} \exp(-K_1 t)$$

$$\frac{dC_B}{dt} = K_1 C_A - K_2 C_B \quad \Rightarrow \quad \frac{dC_B}{dt} = K_1 C_{A0} \exp(-K_1 t) - K_2 C_B$$

$$C_B = C_{Bhom} + C_{BP} \qquad\qquad C_{BP} = A \exp(-K_1 t)$$

$$\downarrow \qquad\qquad\qquad\qquad \downarrow$$

$$\frac{dC_{Bhom}}{dt} = -K_2 C_{Bhom} \qquad -A K_1 \exp(-K_1 t) = K_1 C_{A0}\exp(-K_1 t) + A \exp(-K_1 t)$$

$$C_{Bhom} = B \cdot \exp(-K_2 t) \qquad -A K_1 = K_1 C_{A0} + A K_2$$

$$A = \frac{K_1 C_{A0}}{K_2 - K_1}$$

$$C_B = C_{Bhom} + C_{BP}$$

$$C_B = B \exp(-K_2 t) + \frac{K_1 C_{A0}}{K_2 - K_1} \exp(-K_1 t)$$

initial
condition $\qquad C_B(t=0)=0 \qquad\qquad 0 = B + \frac{K_1 C_{A0}}{K_2 - K_1}$

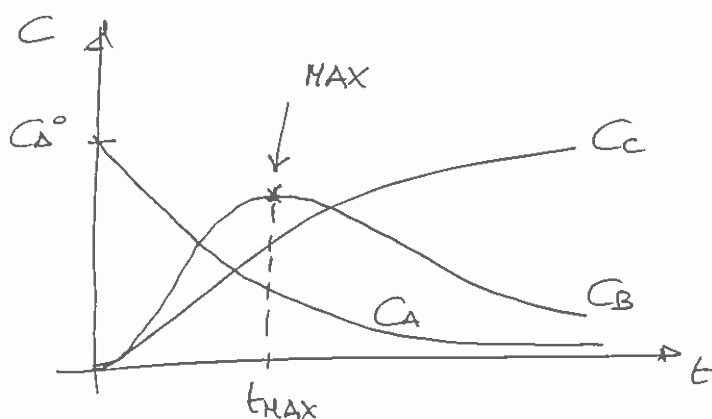$$C_B(t) = \frac{K_1 C_{A0}}{K_2 - K_1} \left(\exp(-K_1 t) - \exp(-K_2 t) \right)$$

$$C_{tot} = C_B + C_A + C_c = \text{const} \implies C_c(t) = C_{tot} - C_A - C_B$$

solution

$$C_A(t) = C_{A0} \exp(-K_1 t)$$

$$C_B(t) = \frac{K_1 C_{A0}}{K_2 - K_1} \left(\exp(-K_1 t) - \exp(-K_2 t) \right)$$

$$C_c(t) = C_A^0 - C_A(t) - C_B(t)$$

$$C_{A0} = 35.7 \; \frac{mol}{m^3}$$

$$\tau = \frac{L}{V} = 3.23 \; s$$

$$\eta_c = \frac{C_c(\tau)}{C_A^0} = \frac{C_c(\tau)}{C_A^0} = 96.8\%$$

$$K_1 = 1.98 \; s^{-1}$$
$$K_2 = 1.86 \; s^{-1}$$

$$C_B(t) = \alpha \left(\exp(-K_1 t) - \exp(-K_2 t) \right) \qquad , \quad \alpha = \frac{K_1 C_{A0}}{K_2 - K_1}$$

$$\frac{dC_B}{dt} = \alpha \left(-K_1 \exp(-K_1 t) + K_2 \exp(-K_2 t) \right) = 0$$

$$K_1 \exp(-K_1 t) = K_2 \exp(-K_2 t)$$

$$\ln K_1 - K_1 t = \ln K_2 - K_2 t$$

$$t_{MAX} = \frac{\ln \frac{K_2}{K_1}}{K_2 - K_1} = \cdots = \frac{\ln \frac{K_1}{K_2}}{K_1 - K_2} \quad \Big| \; \text{maximum position}$$

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