PRACTICAL SESSION 1

EX. 1

CONSTANT VOLUME BATCH REACTOR

$\rho = \text{const}$ $\quad\quad A \rightarrow B \quad\quad k = 0.01\ s^{-1}$

$C_A^\circ = 2\ \frac{mol}{l}$

$$r = k C_A \quad \begin{cases} R_A = -k C_A \\ R_B = k C_A \end{cases} \quad\quad \begin{cases} \frac{dC_A}{dt} = -k C_A \\ \frac{dC_B}{dt} = k C_A \end{cases}$$

$$\frac{dC_A}{dt} = -k C_A \Rightarrow -C_A^\circ \frac{dX}{dt} = -k C_A^\circ (1-X)$$

$$\begin{cases} \frac{dX}{dt} = k(1-X) \\ X(t=0) = 0 \end{cases} \longrightarrow \frac{dX}{X-1} = -k\,dt$$

$$\ln \frac{X-1}{(X-1)_0} = -kt$$

$$\frac{X-1}{-1} = -kt$$

$$\boxed{X = 1 - \exp(-kt)}$$

$$X(\tau) = 1 - \exp(-k\tau)$$

$$\boxed{\tau = -\frac{1}{k} \ln(1-X)}$$

$\tau(X = 90\%) = 230\ s$

$\tau(X = 99.9\%) = 691\ s$

EX 2.

CONSTANT VOLUME BATCH REACTOR

$A \rightarrow B \qquad r = k C_A^{\mu}, \quad \mu \neq 1$

$$\frac{dC_A}{dt} = -k C_A^{\mu} \Rightarrow -C_A^{0}\frac{dX}{dt} = -k C_{A0}^{\mu}(1-X)^{\mu}$$

$$\begin{cases} \dfrac{dX}{dt} = k C_{A0}^{\mu-1}(1-X)^{\mu} \\ X(t=0) = 0 \end{cases}$$

$$(1-X)^{-\mu} dX = k C_{A0}^{\mu-1} dt$$

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

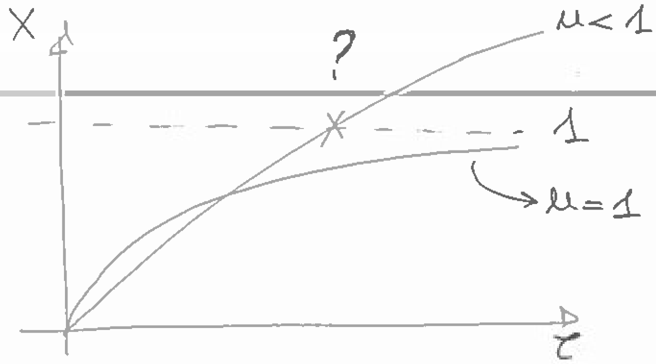
$$\int (1-X)^{-\mu} dX = \underset{\substack{\uparrow \\ y \overset{\text{def}}{=} 1-X}}{\dots\dots} = -\int y^{-\mu} dy = -\left[\frac{y^{-\mu+1}}{-\mu+1}\right]$$

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

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

$$\tau(X) = \frac{(1-X)^{-\mu+1} - 1}{k C_{A0}^{\mu-1}(\mu-1)}$$

$$\begin{cases} \mu = 1/2 & \tau(90\%) = 193\ s \\ \mu = 2 & \tau(90\%) = 950\ s \end{cases}$$



! BE CAREFUL

EX. 3

CSTR at constant density

$$A + B \rightarrow C \qquad r = k C_A C_B$$

$$\begin{cases} k = 0.05 \ \frac{l}{mol\, s} \\ C_{A0} = 3 \ \frac{mol}{l} \\ C_{B0} = 4 \ \frac{mol}{l} \end{cases}$$

$$F_A^\circ - F_A + R_A V = 0 \implies Q(C_{A0} - C_A) + R_A V = 0$$

$$Q\left(C_{A0} - C_{A0}(1-X)\right) - k C_{A0}(1-X) C_{A0}(\vartheta_B^\circ - X) V = 0$$

$$Q C_{A0} X - k C_{A0}^2 (1-X)(\vartheta_B^\circ - X) V = 0 \qquad \tau \overset{def}{=} \frac{V}{Q}$$

$$\vartheta_B^\circ = \frac{C_B^\circ}{C_A^\circ}$$

$$X - k C_{A0}(1-X)(\vartheta_B^\circ - X)\tau = 0$$

$$\tau = \frac{X}{k C_{A0}(1-X)(\vartheta_B^\circ - X)} = \ldots = \frac{X}{k(1-X)(C_B^\circ - C_{A0} X)}$$

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

Observation

$$\begin{cases} C_B = C_{B0} - C_{A0} X \\ C_A = C_{A0} - C_{A0} X \end{cases}$$

$$C_B - C_A = C_{B0} - C_{A0} \overset{def}{=} \Delta C_0 = \text{const}$$

$$C_B = C_A + \Delta C_0$$

$$C_B^\circ = C_A^\circ + \Delta C_0 \implies C_B^\circ - X C_A^\circ = \ldots = C_A^\circ(1-X) + \Delta C_0$$

$$\tau = \frac{X}{k(1-X)\left(C_A^\circ(1-X) + \Delta C_0\right)}$$

EX. 4

CONSTANT DENSITY CSTR

$$A \rightleftharpoons B \qquad r = k_f C_A - k_b C_B \qquad \begin{cases} k_f = 0.5 \ \text{min}^{-1} \\ k_b = 0.1 \ \text{min}^{-1} \end{cases}$$

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

<u>Equilibrium</u>

$$k_f C_{Aeq} = k_b C_{Beq}$$

$$k_f \cancel{C_{A0}} (1 - X_{eq}) = k_b \cancel{C_{A0}} X_{eq}$$

$$X_{eq} = \frac{k_f}{k_f + k_b} \qquad X_{eq} = 5/6 > 50\% \ \checkmark$$

<u>Residence time</u>

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

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

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

$$X - (k_f(1-X) - k_b X)\tau = 0$$

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

EX. 5

CSTR with non constant density

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

$$\begin{cases} C_A^\circ = 3 \, \frac{\text{mol}}{\ell} \\ C_B^\circ = 0 \\ F_A^\circ = 0.2 \, \frac{\text{mol}}{s} \end{cases}$$

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

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

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

$\overset{!}{=} \dot{Q}_0 (1 + 2X)$

$$\left| \begin{array}{l} C_j = C_{A0} \frac{\vartheta_j^\circ + \nu_j X}{1 + \varepsilon X} \gamma^* \\ \gamma^* = \frac{T^\circ P}{T P_0} = \ldots = 1 \\ \varepsilon = \frac{F_A^\circ}{F_{tot}^\circ} \delta = 1 \cdot (3 - 1) = 2 \end{array} \right.$$

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

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

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

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

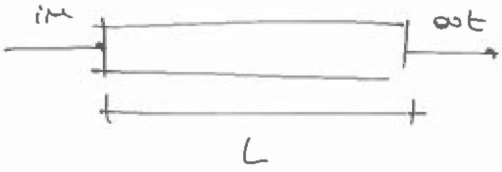
$X - K C_{A0} \frac{(1 - X)^2}{(1 + 2X)^2} \tau = 0$

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

$\tau(95\%) = 734.7 \text{ min}$

EX 6

REACTIONS IN SERIES IN A PFR (constant density)



$L = 100\ m$

$d = 0.08\ m$

$T = 750\ °C$

$P = 3\ bar$

$\dot{F}_A^\circ = 20\ \frac{kmol}{h}$

$\dot{F}_B^\circ = \dot{F}_C^\circ = 0$

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

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \qquad \begin{cases} r_1 = k_1 C_A \\ r_2 = k_2 C_B \end{cases}$$

$$\begin{cases} \dfrac{dC_A}{dt} = -k_1 C_A \\ \dfrac{dC_B}{dt} = k_1 C_A - k_2 C_B \\ \dfrac{dC_C}{dt} = k_2 C_B \end{cases} + \ ICs \begin{cases} C_A(0) = C_A^\circ = \dot{F}_A^\circ / \dot{Q} \\ C_B(0) = C_B^\circ = 0 \\ C_C(0) = C_C^\circ = 0 \end{cases}$$

$$\frac{dC_A}{dt} = -k_1 C_A \implies C_A = C_{A0} \exp(-k_1 t)$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \implies \frac{dC_B}{dt} = k_1 C_{A0} \exp(-k_1 t) - k_2 C_B$$

$$C_B = C_{B\,hom} + C_{Bp} \qquad C_{Bp} = A \exp(-k_1 t)$$

$$\frac{dC_{B\,hom}}{dt} = -k_2 C_{B\,hom} \qquad -Ak_1 \exp(-k_1 t) = k_1 C_{A0} \exp(-k_1 t) + A \exp(-k_1 t) k_2$$

$$C_{B\,hom} = B \cdot \exp(-k_2 t) \qquad -Ak_1 = k_1 C_{A0} + A k_2$$

$$A = \frac{k_1 C_{A0}}{k_2 - k_1}$$

$$C_B = C_{B\,hom} + C_{Bp}$$

$$C_B = B \exp(-k_2 t) + \frac{k_1 C_{A0}}{k_2 - k_1} \exp(-k_1 t)$$

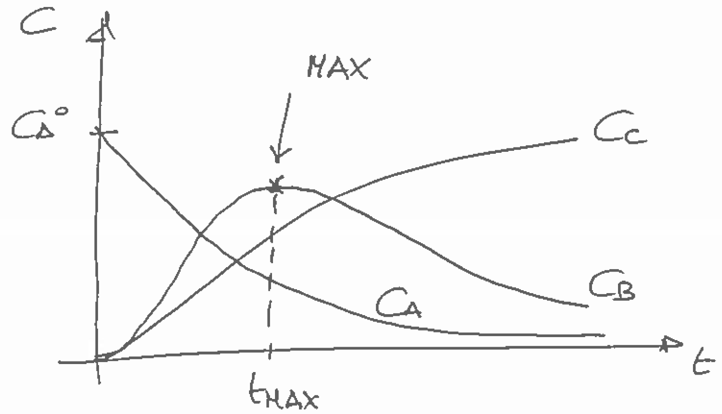
initial condition $\quad C_B(t=0)=0 \qquad 0 = \beta + \frac{k_1 C_{A0}}{k_2-k_1}$

$$C_B(t) = \frac{k_1 C_{A0}}{k_2-k_1}\left(\exp(-k_1 t) - \exp(-k_2 t)\right)$$

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

solution

$$\begin{cases} C_A(t) = C_{A0}\exp(-k_1 t) \\ C_B(t) = \dfrac{k_1 C_{A0}}{k_2-k_1}\left(\exp(-k_1 t) - \exp(-k_2 t)\right) \\ C_C(t) = C_A^0 - C_A(t) - C_B(t) \end{cases}$$



$$\begin{cases} C_{A0} = 35.7 \ \frac{mol}{m^3} \\ \tau = \frac{L}{v} = 3.23\,s \\ \eta_C = \frac{C_C(\tau)}{C_A^0} = \frac{C_C(\tau)}{C_A^0} = 96.8\% \\ k_1 = 1.49\ s^{-1} \\ k_2 = 1.86\ s^{-1} \end{cases}$$

$$C_B(t) = \alpha\left(\exp(-k_1 t) - \exp(-k_2 t)\right), \quad \alpha = \frac{k_1 C_{A0}}{k_2-k_1}$$

$$\frac{dC_B}{dt} = \alpha\left(-k_1\exp(-k_1 t) + k_2\exp(-k_2 t)\right) = 0$$

$$k_1\exp(-k_1 t) = k_2\exp(-k_2 t)$$

$$\ln k_1 - k_1 t = \ln k_2 - k_2 t$$

$$t_{MAX} = \frac{\ln\frac{k_2}{k_1}}{k_2-k_1} = \dots = \frac{\ln\frac{k_1}{k_2}}{k_1-k_2}$$

! maximum position