Demoövn. 2

Tis LV2

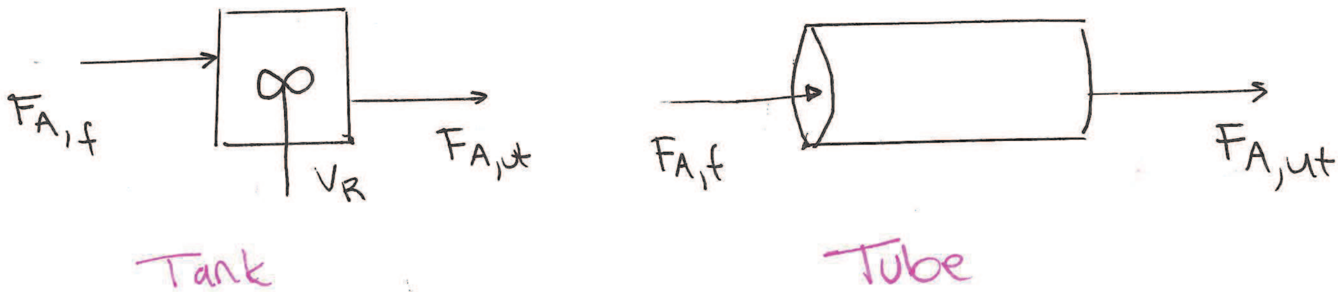
Molbalans - ideal reaktorer

$\boxed{3}$ $A \rightarrow B$ $\quad X_A = 80\%$

Sökt: volym för en tank- resp. tubreaktor

$r = kC_A \qquad k = 0.1\ s^{-1}$

$q = 4 \cdot 10^{-3}\ m^3/s$



Tank

MB: $F_{A,f} - F_{A,ut} + \nu_A r V_R = \frac{dN_A}{dt} = 0$ steady-state

$$F_{A,f} - F_{A,f}(1-X) - kC_A V_R = 0$$

$$V_R = \frac{F_{A,f}X}{kC_A} = \frac{F_{A,f} \cdot X}{kC_{A,f}(1-X)} = \frac{q \cdot \cancel{C_{A,f}} \cdot X}{k\,\cancel{C_{A,f}}(1-X)} =$$

$\rightarrow V_R = 0.16\ m^3$

Tube

$$F_A - (F_A + dF_A) + \nu_A r\, dV_R = 0$$

$$-d(F_{A,f}(1-x)) - kC_A\, dV_R = 0$$

$$F_{A,f}\, dx - kC_A\, dV_R = 0$$

$$dV_R = \frac{F_{A_f}\, dx}{kC_{A,f}(1-x)} \longrightarrow V_R = \frac{q C_{A,f}}{kC_{A,f}} \int_0^{x=0.8} \frac{dx}{1-x}$$

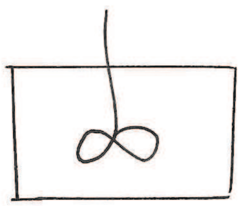
$$V_R = \frac{q}{k}\left[-\ln(1-x)\right]_0^{0.8} = 0.064\ m^3$$

$$\Longrightarrow V_{tube} < V_{tank}\ !$$

Reaktorkapacitet

$\boxed{6}$ $A + B \rightleftharpoons S + R$

$T = 100\ °C$	$K = 2.94$
$y_A^\circ = 30\%$	$\rho = 1000\ kg/m^3$
$y_B^\circ = 15\%$	$t_{empty+fill} = 1h$
$y_S^\circ = 55\%$	$r = k_1\left(C_A C_B - \frac{C_R C_S}{K}\right)$
$x_B = 35\%$	in a batch reactor



no flow in/out

Sökt: V_R - 50 ton R/dag

$$MB: \nu_B r V_R = \frac{dN_B}{dt}$$

$$① \quad -k_1\left(C_A C_B - \frac{C_R C_S}{K}\right) V_R = \frac{dN_B}{dt}$$

$$C_A = C_A^0 - C_B^0 X_B = C^0 (y_A - y_B X_B)$$

$$C_B = C^0 y_B (1 - X_B)$$

$$C_R = C^0 y_B X_B$$

$$C_S = C^0 (y_S + y_B X_B)$$

$$① \longrightarrow k_1 \left[C^0 (y_A - y_B X_B) C^0 (y_B - y_B X_B) - \frac{C^0 y_B X_B \cdot C_0 (y_S + y_B X_B)}{K} \right] / \cancel{N}_B = \frac{dN_B}{dt}$$

$$C^{0^2} k_1 \left((y_A - y_B X_B)(y_B - y_B X_B) - \frac{y_B X_B (y_S + y_B X_B)}{K} \right) = C^0 \frac{dX_B}{dt}$$

$$k_1 dt = \frac{dX_B}{C^0 \left(\underbrace{\left(y_B - \frac{y_B}{K}\right)}_{A} X_B^2 - \underbrace{\left(y_A + y_B + \frac{y_S}{K}\right)}_{B} X_B + \underbrace{y_A}_{C} \right)} \qquad AX^2 + BX + C$$

$$C^0 k_1 T = \left[\frac{1}{\sqrt{\Delta}} \ln \left(\frac{2AX - B\sqrt{\Delta}}{2AX + B\sqrt{\Delta}} \right) \right]_0^{X_B = 0.35}$$

$$\Delta = B^2 - 4AC \qquad \begin{cases} A = 0.099 \\ B = 0.637 \\ C = 0.3 \\ \Delta = 0.287 \end{cases}$$

$$\Longrightarrow C^0 k_1 T = 2.038$$

T to reach 35%.

$$T = \frac{2.038}{c^{\circ} k_1}$$

$$c^{\circ} = \frac{n^{\circ}}{V_R} = \frac{m^{\circ}}{M V_R} = \frac{\rho}{M} = \frac{1000}{32.7} = 30.58 \ \text{kmol}/\text{m}^3$$

$$M = 0.15 \cdot 60 + 0.3 \cdot 46 + 0.55 \cdot 18 = 32.7 \ \text{kg}/\text{kmol}$$

$$T = \frac{2.038}{3.05 \cdot 10^{-2} \cdot 30.58} = 2.18 \ h$$

In one day: $\frac{24}{3.18} = 7.536$ batches can be produced.

Production per batch: $\frac{50}{7.536} = 6.635$ ton (6635 kg)

$$V_R = \frac{n_R}{c_R} = \frac{m_R}{\underbrace{M_R c_R}_{M_R c_R^{\circ} X_B}} = \frac{6635}{88 \cdot 0.35 \cdot 0.15 \cdot 30.58} = 46.96 \ m^3$$

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$A \longmapsto B + C$

$F_{A,f} = 100 \text{ mol A/h}$ (pure A in the feed)

$k_1 = 10 \ (\text{mol/dm}^3)^{0.5} \ h^{-1}$

$k_2 = 16 \ \text{dm}^3/\text{mol}$

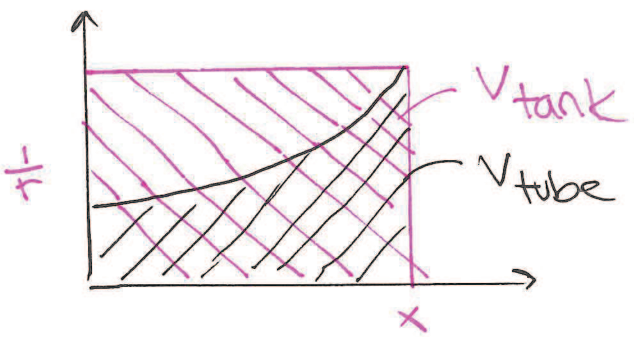
$C_{A,f} = 0.25 \ \text{mol/dm}^3$

$$r = \frac{k_1 C_A^{0.5}}{1 + k_2 C_A} \qquad X = 90\%$$

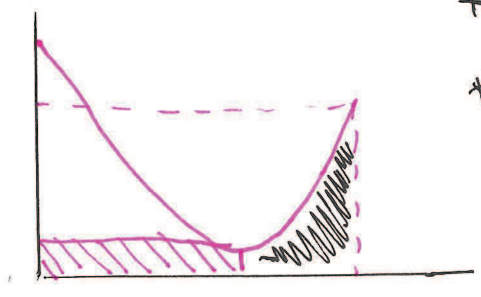
Sökt: V_R minimum!

Tube: $V = F_{A,f} \int_0^X \frac{dX}{r(X)}$

Tank: $V = F_{A,f} \frac{X}{r(X)}$



Plot $\frac{1}{r}$ mot X



* need two reactors in series
* one tank from X=0 to X_1

One tube $X_1 \rightarrow 0.9$

X_1:

$$\frac{dr}{dx} = 0 = \frac{d}{dx}\left(\frac{k_1 (C_A^\circ (1-x))^{0.5}}{1 + k_2 (C_A^\circ (1-x))}\right)$$

$$\frac{\frac{1}{2}\frac{k_1}{\sqrt{C_A^\circ (1-x)}}\left(1 + k_2 C_A^\circ (1-x) - k_1 \sqrt{C_{A_0}(1-x)}\ k_2\right.}{(1 + k_2 C_A^\circ (1-x))^2} = 0$$

$$0.5 k_1 + 0.5 k_1 k_2 C_{A_0}(1-x) = k_1 k_2 C_{A_0}(1-x)$$

$$\longrightarrow X_1 = 0.75$$

V_{tank}? $V = F_{A_f} \frac{X_1}{r} = \frac{F_{A_f} X_1 (1 + k_2 C_{A_1})}{k_1 \underbrace{\sqrt{C_{A_1}}}}$ — $C_{A_0}(1-X) = \frac{1}{16}$

$$V = \frac{100 \times 0.75 (1 + \frac{16}{16})}{10\sqrt{\frac{1}{16}}}$$

$$V = 60\,L$$

V_{tube}? $X = 0.75 \longrightarrow X = 0.9$

$$V = F_{A_f} \int_{0.75}^{0.9} \frac{dx}{r} = F_{A_f} \int_{0.75}^{0.9} \frac{1 + k_2 C_A}{k_1 \sqrt{C_A}}\, dX$$

$$V = \frac{F_{A_f}}{k_1} \int_{0.75}^{0.9} \frac{1}{\sqrt{C_A^\circ (1-x)}}\, dX + \frac{F_{A_f} k_2}{k_1} \int_{0.75}^{0.9} \sqrt{C_{A_0}(1-x)}\, dX$$

$$V = \frac{F_{A,f}}{k_1}\left[-\frac{2}{\sqrt{C_A^o}}\sqrt{1-X}\right]_{0.75}^{0.9} + \frac{F_{A,f}k_2}{k_1}\left[-\frac{2\sqrt{C_A^o}}{3}(1-X)^{3/2}\right]_{0.75}^{0.9}$$

$$V = \frac{100\cdot 2}{10\sqrt{0.25}}\left(\sqrt{0.25}-\sqrt{0.1}\right) + \frac{100\cdot 16}{10}\cdot\frac{2\sqrt{0.25}}{3}\left(0.25^{3/2}-0.1^{3/2}\right)$$

$$V = 12.3\ L$$