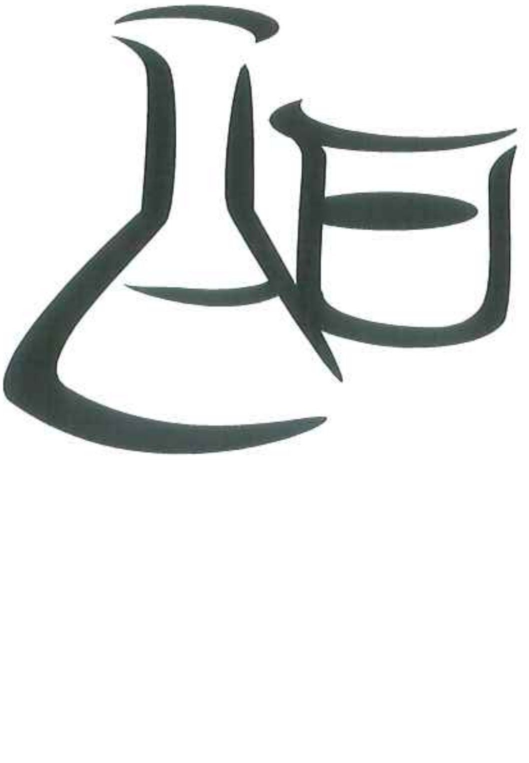
Studienämnden Kf / Kb

Februari 2009

Kemisk ReaktionsTeknik

Lösningar



Av: Patrik "Putte" Andersson kf-06

1.2) $A + B \rightarrow C$ $\quad -r = kC_AC_B \quad k = 1.2\,e^{-3}\,mol/s$

C_B är i stort överskott ⇒ C_B är konstant

$$C_B = \frac{m}{MV} = \frac{\rho}{M} = \frac{1000}{18} = 55.56$$

Molbalans ideal tankreaktor

$$F_{A0} - F_{A0}(1-x) = kC_AC_BV \qquad t = \frac{V}{q} = 600\,s = \tau$$

$$qC_{A0} - qC_{A0}(1-x) = kC_BVC_{A0}(1-x)$$

$$x = \frac{tkC_B}{1+tkC_B} = 0.9756 \approx 0.98$$

b) $C_{A1} = 0.002$ början

$C_{A2} = 0.005$ slut

$C_{Af} = 0.99\,C_{A2} \approx 0.005$

Molbalans

$$\frac{C_{A0}}{\tau} - \frac{C_A}{\tau} - kC_AC_B = \frac{dC_A}{dt}$$

$$t = \int_{C_{A1}}^{C_{Af}} \frac{dC_A}{\frac{C_{A0}}{\tau} - \frac{C_A}{\tau} - kC_AC_B}$$

$$t = -\frac{1}{\frac{1}{\tau} + kC_B}\left[\ln\left(\frac{C_{A0}}{\tau} - C_A\left(\frac{1}{\tau} + kC_B\right)\right)\right]_{C_{A1}}^{C_{Af}} \approx \underline{\underline{19.3\ s}}$$

1.3) $A + B \rightarrow C$ $V = 6\,m^3$ $r = kC_A$ $F_{A0} = 4\ kmol/s$

$k = 2.63\,E^{-3}$ $q = 0.4\ m^3/min$

$$t = \frac{6 \cdot 60}{0.4} = 900\ s$$

Molbalans semisatsreaktor

$$F_{A0} - rV = \frac{dN_A}{dt} \qquad N_A = C_A \cdot V \Rightarrow$$

$$t = \int_0^{N_A} \frac{dN_A}{F_{A0} - kN_A} = -\frac{1}{k} \ln\left(\frac{F_{A0} - kN_A}{F_{A0}}\right)$$

$$\Rightarrow N_A = \frac{F_{A0} - F_{A0}e^{-tk}}{k} = 9.18\ kmol$$

$$C_A = N_A/V = \underline{\underline{1.53\ kmol/m^3}}$$

b) $C_{A0} = 4\ kmol/m^3$

Molbalans tankreaktor

$$F_{A0} - F_A = kC_AV \qquad F = q \cdot C$$

$$C_A = \frac{F_{A0}}{q + kV} = \underline{\underline{1.188\ kmol/m^3}}$$

1.5 } $A \to B$ $r = kC_A$ $k = 0.1\ m^3/s\ kg\ kat$ $q = 0.1\ m/s$

$C_{A0} = 500\ mol/m^3$ $V_r = 5\ m^3$ $W = 0.5\ kg$ $V_0 = 0.5\ m^3$

Molbalans satsreaktor

påfyllnad efter katalysator

$$qC_{A0} - kC_A W = \frac{dV \cdot C_A}{dt}$$

$$\frac{dV}{dt} = q \Rightarrow V_r = V_0 + qt \Rightarrow t = 45\ s$$

$$\frac{dV_r \cdot C_A}{dt} = C_{A0}\frac{dV_r(1-x)}{dt} = C_{A0}\left((1-x)\frac{dV_r}{dt} - V_r\frac{dX}{dt}\right)$$

$$\Rightarrow qC_{A0} - kC_{A0}(1-x)W = C_{A0}\left((1-x)q - V_r\frac{dX}{dt}\right)$$

$$\Rightarrow q - kW(1-x) - (1-x)q = -V_r\frac{dX}{dt}$$

$$\Rightarrow -\int\frac{dt}{V_0+qt} = \int\frac{dX}{q-kW(1-x)-(1-x)q} = \int\frac{dX}{kW - x(q+kW)}$$

$$\underbrace{\frac{1}{q}\ln\left(\frac{qt+V_0}{V_0}\right)}_{\alpha} = -\underbrace{\frac{1}{q+kW}}_{\beta}\ln\left(\frac{kW - x(q+kW)}{kW}\right)$$

$$x = \frac{kW - kWe^{\alpha/\beta}}{kW} = 0.3227 \approx \underline{\underline{0.327}}$$

2.1) $A \xrightarrow[R_1]{} B \xrightarrow[R_2]{} C$ $F_{A0} = 1 \text{ mol/s}$ $C_{A0} = 0.001$

Molbalans tankreaktor

$$qC_{A0} - qC_A - k_1 C_A V = 0 \Rightarrow C_A = \frac{qC_{A0}}{q + k_1 V} = 200 \text{ mol/m}^3$$

$$-qC_B + k_1 C_A V - k_2 C_B V = 0$$

$$\Rightarrow C_B = \frac{k_1 V C_{A0}}{(q + k_1 V)(q + k_2 V)} = 400 \text{ mol/m}^3$$

$$C_C = C_{A0} - C_A - C_B = \underline{\underline{400 \text{ mol/m}^3}}$$

2.2}

$A \rightarrow B \qquad \Delta H_1 = -100 \text{ kJ/mol} \qquad r_1 = k_1 C_A$

$A \rightarrow C \qquad \Delta H_2 = -200 \text{ kJ/mol} \qquad r_2 = k_2 C_A$

$$k = A \exp\left(\frac{-E_A}{T}\right) \quad (1) \qquad A_1 = 0.4\, s^{-1} \qquad A_2 = 300\, s^{-1}$$

Molbalans

$$q C_{A0} - q C_{A0}(1-x) - (k_1 + k_2) V C_{A0}(1-x) \Rightarrow$$

$$x = \frac{(k_1 + k_2) V}{q + (k_1 + k_2) V} \quad (2)$$

Vårmebalans

$$\int_{T_0}^{T_r} q \rho C_p \, dT - \int_{T_r}^{T} q \rho C_p \, dT + (\Delta H_1 k_1 + \Delta H_2 k_2) C_{A0}(1-x) V$$

$$T_r = T \Rightarrow q \rho C_p (T - T_0) + (\Delta H_1 k_1 + \Delta H_2 k_2) C_{A0}(1-x) V = 0$$

$$T = T_0 - \frac{C_{A0}(1-x) V (k_1 \Delta H_1 + k_2 \Delta H_2)}{\rho C_p q} \quad (3)$$

Iterera

$$\text{Gissa } T \xrightarrow{(1)} k_1 \,\&\, k_2 \xrightarrow{(2)} x \xrightarrow{(3)} T$$

$\underline{\underline{T = 405 \text{ K}}} \qquad \underline{\underline{k_1 \approx 0.00104}} \qquad \underline{\underline{k_2 \approx 0.002029}} \qquad \underline{\underline{x = 0.75}}$

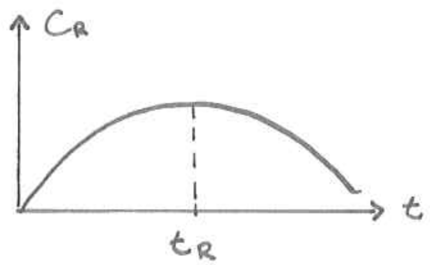
2.3) $A + B \rightarrow R \rightarrow 2S$ $\quad r_A = -k_1 C_A \quad r_R = -k_2 C_R$

$P_R = 100$ kg/h $\quad C_{S0} = 0$

$t_{cykel} = t_{reaktion} + t_{övrigt} \quad (t_c = t_R + t_ö$

$t_{reaktion}$ väljs så att $C_{Rt_R} = C_{RMAX}$

$C_{R0} = 0$ R bildas i reaktion 1 o förbrukas i reaktion 2
A tar slut ⇒ bildning av R minskar medan
reaktion 2 fortgår ⇒ erhålls ett C_{RMAX} för
en viss tid t_R



$t_R \Rightarrow \frac{dC_R}{dt} = 0$

Massbalanser

$$\frac{dN_A}{dt} = -k_1 C_A V$$

$$\frac{dN_B}{dt} = -k_1 C_A V$$

$$\frac{dN_R}{dt} = V(k_1 C_A - k_2 C_R)$$

$$\frac{dN_S}{dt} = 2 k_2 C_R V$$

$$\frac{dN_R}{dt} = \frac{d(C_R V)}{dt} = \not{V}\frac{dC_R}{dt} = \not{V}(k_1 C_A - k_2 C_R) \qquad (*)$$

$$\frac{dN_A}{dt} = V\frac{dC_A}{dt} = -k_1 C_A V$$

$$\int_{C_{A0}}^{C_A} \frac{dC_A}{C_A} = -k_1 \int_0^t dt \quad \Rightarrow \quad C_A = C_{A0}\exp(-k_1 t) \qquad (**)$$

$$\therefore \quad C_{RMAX} = \frac{k_1}{k_2} C_{A0}\exp(-k_1 t)$$

$$(*) \text{ o } (**) \Rightarrow \quad \frac{dC_R}{dt} = k_1 C_{A0}\exp(-k_1 t) - k_2 C_R \quad \Rightarrow$$

$$\frac{dC_R}{dt} + k_2 C_R = k_1 C_{A0}\exp(-k_1 t)$$

Ordinär linjär differentialekvation $\Rightarrow$ Beta $\Rightarrow$

$y' + f(x)\,y = g(x) \qquad f(x) = a =$ konstant $\Rightarrow$

$$y(x) = \frac{A\exp(kx)}{k-a} + C\exp(ax)$$

$A = k_1 C_{A0}$

$k = -k_1$

C integreras fram

$$\left.\begin{matrix} \\ \\ \end{matrix}\right\} \quad C_R(t) = \frac{k_1 C_{A0}\exp(-k_1 t)}{k_2 - k_1} + C\exp(-k_2 t)$$

Begynnelsevärden:

$$C_R(0) = \frac{k_1 C_{A0}}{k_2 - k_1} + C = 0 \Rightarrow C = -\frac{k_1 C_{A0}}{k_2 - k_1} \Rightarrow$$

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

$$\frac{dC_R}{dt} = 0 \Rightarrow$$

$$\frac{k_1 C_{A0}}{k_2 - k_1}\left(k_2 \exp(-k_2 t) - k_1 \exp(-k_1 t)\right) = 0 \Rightarrow$$

$$t_R = 835\ s = 13.92\ min$$

$$C_R(t_R) = 0.6\ kmol/m^3$$

$$t_C = t_R + t_ö = 43.9\ min$$

$$P_R = \frac{m_{R\,cykel}}{t_{cykel}} = \frac{C_{R\,MAX}\, V_R \cdot M_R}{t_C} \Rightarrow$$

$$V_R = \frac{P_R t_C}{C_{R\,MAX} M_R} \qquad M_R = M_A + M_B \quad ty \quad A + B \rightarrow R$$

$$M_R = 98\ kg/mol \Rightarrow V_R = \underline{\underline{1.24\ m^3}}$$

2,4} $E \rightarrow S \qquad r_1 = k_1 C_E \qquad k_1 = 0.496\,E^{-3}$

$S \rightarrow B + C \qquad r_2 = k_2 C_E \qquad k_2 = 0.117\,E^{-3}$

$F_{E0} = 2\ \text{mol/s}$ Gasfas, ty $T = 700°C$

Molbalans

$$\frac{dF}{dW} = -r_1 - r_2 \Rightarrow F_{E0}\frac{dX}{dW} = C_E(k_1 + k_2)$$

$$C_E = \frac{F_{E0}(1-x)}{F_{TOT}}\frac{P}{RT}$$ [redacted]

$$\Rightarrow \frac{dX}{dW} = \frac{P}{RT}\frac{(1-x)}{F_{TOT}}(k_1 + k_2)$$ Vet ej F_{TOT} !

Reaktion 1

Andel E som förbrukas: $\frac{r_1}{r_1 + r_2} = \frac{k_1}{k_1 + k_2} = \alpha$

Reaktion 2

Andel E som förbrukas: $\frac{k_2}{k_1 + k_2} = \beta$

$$\left.\begin{aligned} F_E &= F_{E0}(1-x) \\ F_S &= F_{E0} X \alpha \\ F_{H_2} &= F_{E0} X \alpha \\ F_B &= F_{E0} X \beta \\ F_C &= F_{E0} X \beta \end{aligned}\right\} \quad F_{TOT} = F_{E0}\Big((1-x) + 2X\alpha + 2X\beta\Big)$$

$$= F_{E0}\left(1 - x + 2X\left(\frac{k_1 + k_2}{k_1 + k_2}\right)\right)$$

$$= F_{E0}(1 + X)$$

$$\frac{dX}{dW} = \frac{(1-X)}{(1+X)} \frac{P}{RTF_{E0}} (k_1 + k_2)$$

$$\int \frac{(1+x)}{(1-x)} = \frac{P}{RT} \cdot \frac{W}{F_{E0}} \cdot (k_1 + k_2) \approx 1.23$$

$$\Rightarrow -x - 2\ln(1-x) = 1.23$$

$$\Rightarrow x = 0.5997$$

$$F_E = F_{E0}(1-x) = 0.8$$

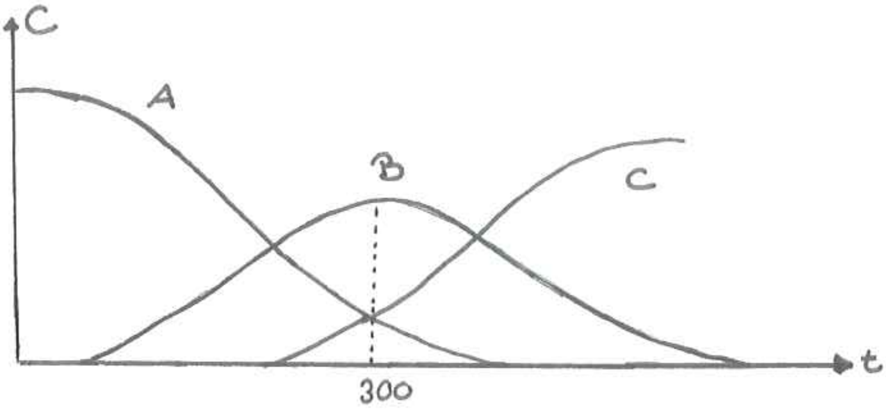
$$F_S = F_{E0}\, x\, \alpha = 0.97$$

$$F_{H_2} = F_{E0}\, x\, \alpha = 0.97$$

$$F_B = F_{E0}\, x\, \beta = 0.23$$

$$F_C = F_{E0}\, x\, \beta = 0.23$$

2.6)



Satsreaktor: $\frac{10\,g \text{ katalysator}}{1\,dm^3 \text{ reaktor}} \Rightarrow \rho_B = \frac{10\,kg \text{ katalysator}}{m^3 \text{ reaktor}}$

Tubreaktor: $\frac{dF_A}{dV} = -r_i \rho_T = \frac{dC_A}{d\tau}$ om q är konstant

Tiden (t) i satsreaktorn är propotionell mot uppehållstiden (τ) i tubreaktorn: $t_{opt} \propto \tau_{opt}$

$\Rightarrow t_{opt} \cdot \rho_B = \tau_{opt} \rho_T \Rightarrow \tau_{opt} = 300 \cdot \frac{10}{2000} = \underline{\underline{1.5\,min}}$

$F_B = 16.67 \frac{mol}{min}$ $C_B = 0.57 \frac{mol}{dm^3}$ vid τ_{opt}

$q = \frac{F_B}{C_B} = 29.24 \frac{dm^3}{min}$ $V = q \cdot \tau_{opt} = 43.86\,dm^3$

$m_{cat} = \rho_T \cdot V = \underline{\underline{87.72}}\,kg$

2.7)

$$A \xrightarrow{k_1} B \qquad -r_{A1} = k_1 C_A \qquad k_1 \text{ beror av } T$$

$$A \xrightarrow{k_2} C \qquad -r_{A2} = k_2 C_A \qquad k_2 \text{ beror av } T$$

Molbalans för A:

$$q\, C_{A0} X = (k_1 + k_2) C_{A0} (1-x) V$$

$$\Rightarrow \quad X = \tau (k_1 + k_2)(1-x) \qquad (1)$$

Molbalans för B:

$$F_B = k_1 C_A V$$

$$\Rightarrow \quad F_B = k_1 C_{A0} (1-x) V \qquad (2)$$

Värmebalans

$$-\sum F_{i0} \int_{T_0}^{T} C_p \, dT - k_1 C_A V \Delta H_1 - k_2 C_A V \Delta H_2 - U A (T - T_k) = 0$$

$$A = \frac{-q \rho C_p (T - T_0) + k_1 C_{A0} (1-X) V \Delta H_1 + k_2 C_{A0} (1-X) V \Delta H_2}{U (T - T_k)} \qquad (3)$$

Sätt in (1) i (2) och "plotta" F_B mot T. Ta fram T_{opt} vid F_{Bmax}. Sätt in i (1) för att få fram X_{opt}.

Sätt in i (3) för att få fram A

$$A = \underline{\underline{10.4 \ m^2}}$$

3.3} $A \rightarrow R \qquad -r_A = kC_A \qquad k = 0.307 \text{ min}^{-1}$

$$\frac{dC_A}{dt} = kC_A \Rightarrow C_A = C_{A0}\exp(-kt)$$

$$\langle C_A \rangle = \int C_A E(t)$$

$$E(t) = \frac{C_s}{\int C_s} \qquad \int C_s = \frac{5}{2}\cdot 3 + \frac{5}{2}\cdot 8 + \frac{5}{2}\cdot 10 + \frac{5}{2}\cdot 9 + \frac{5}{2}\cdot 6 + \frac{5}{2}\cdot 3 + \frac{5}{2}$$

$$\Rightarrow E(t) = \frac{C_s}{100} \Rightarrow \langle C_A \rangle = C_{A0}\int \frac{C_s}{100}\exp(-kt)$$

t	$C_s/100 \cdot \exp(-kt)$
0	0
5	0.0064
10	0.0023
15	5 E^{-4}
20	8.619 E^{-5}
25	9.285 E^{-6}
30	E^{-6}
35	0

$$\Rightarrow \langle C_A \rangle = C_{A0} \cdot 0.04669$$

$$\Rightarrow \frac{\langle C_A \rangle}{C_{A0}} \approx 4.7\%$$

t	$t\,E(t)$
0	0
5	0.15
10	0.5
15	0.75
20	0.8
25	0.5
30	0.2
35	0

$$\Rightarrow \langle t \rangle = 15 \text{ min}$$

$$q\frac{dC_A}{dV} = -kC_A \Rightarrow \ln\frac{C_A}{C_{A0}} = \frac{-k}{q}V$$

$$\Rightarrow \frac{C_A}{C_{A0}} = \exp(-kt) \approx \underline{\underline{1\%}}$$

3.4) $2A \rightarrow B$ $r = k\, y_A^2$ $k = 0{,}01$

$$\frac{dy_A}{dt} = k\, y_A^2 \Rightarrow y_A = \frac{y_{A0}}{y_{A0}kt+1} = \frac{1}{kt+1} \quad \text{ty } y_{A0} = 1$$

$$\langle y_A \rangle = \int E(t)\cdot y_A = \int \frac{C_S}{215 + 215kt}$$

t	$E(t)\cdot y_A$
0	0
5	0,022
10	0,051
15	0,057
20	0,031
25	0,015
30	0

$\Rightarrow \langle y_A \rangle = 0.876$

$$\langle t \rangle = \int E(t)\cdot t = \int \frac{C_S \cdot t}{215}$$

t	$E(t)\cdot t$
0	0
5	0.1163
10	0.5581
15	0.9767
20	0.7442
25	0.4651
30	0

$\Rightarrow \langle t \rangle = 14{,}3$ min

3.5}

$$-\frac{dS}{dt} = k \cdot S \Rightarrow S = S_0 \exp(-kt) = e^{-kt}$$

$$t = 3 \Rightarrow S = 1/2 \Rightarrow k = 0.231$$

$$\int E(t)\,dt = E(t) \cdot 5 = 1 \Rightarrow E(t) = 1/5$$

$$\langle S \rangle = \int_0^5 E(t) \cdot e^{-kt} = \frac{1}{5 \cdot 0{,}231}\left[1 - e^{-k \cdot 5}\right]$$

$$\langle S \rangle = \underline{\underline{0{,}59}}$$

3.6} Finns flera sätt att lösa uppgiften

1, Dispersionsmodellen

$$vAC_z - vAC_{z+dz} - D_{ea}A\left(\frac{dc}{dz}\right)_z - D_{ea}A\left(\frac{dc}{dz}\right)_{z+dz} - A\,dz\,kC^2 = 0$$

Dea = effektiva axiella dispersionskoefficienten

$$C_{z+dz} = C_z + \left(\frac{dc}{dz}\right)dz$$

$$\left(\frac{dc}{dz}\right)_{z+dz} = \left(\frac{dc}{dz}\right)_z + \left(\frac{d^2c}{dz^2}\right)dz$$

$$D_{ea}\frac{d^2c}{dz^2} - v\frac{dc}{dz} - kC^2 = 0$$

Randvillkor: ingen dispersion i in och utlopp i reaktorn

$$z = 0 \qquad vC_{Af} = vC_A - D_{ea}\frac{dC_A}{dz}$$

$$z = L \qquad \frac{dc}{dz} = 0 \qquad z^* = \frac{z}{L} \qquad \tau = \frac{L}{v} \qquad \Rightarrow$$

$$\frac{D_{ea}}{vL}\frac{d^2c}{dz^{*2}} - \frac{dc}{dz^*} - k_2\tau c^2 = 0$$

Numerisk lösning av differentialekvation ger:

$$\frac{c_L}{c_f} = f\left(k_2\tau c_f, \frac{D_{ea}}{vL}\right)$$

"closed-closed vessel boundary condition" ger:

$$\frac{\sigma^2}{t^2} = 2\frac{D_{ea}}{vL} - 2\left(\frac{D_{ea}}{vL}\right)^2\left(1 - \exp\left(-\frac{vL}{D_{ea}}\right)\right)$$

$$t = \langle t \rangle = \frac{L}{v} = \tau$$

t och σ^2 fås ur spårämnesförsöket:

$$\langle t \rangle = \int t \cdot E(t) = \int \frac{t \cdot C_s}{100} = 15 \text{ min} = \tau$$

$$\sigma^2 = \int (t-\tau)^2 E(t) = 47.5 \text{ min}^2$$

$$\frac{\sigma^2}{t^2} = 0.2111 = 2\frac{D_{ea}}{vL} - 2\left(\frac{D_{ea}}{vL}\right)^2\left(1 - \exp\left(\frac{-vL}{D_{ea}}\right)\right)$$

$\exp\left(\frac{-vL}{D_{ea}}\right)$ försummas $\Rightarrow$

$$\left(\frac{D_{ea}}{vL}\right)^2 = \frac{D_{ea}}{vL} - \frac{0.2111}{2} \Rightarrow$$

$$\frac{D_{ea}}{vL} = 0.5 \pm 0.38 = Pe^{-1}$$

$Pe^{-1} = 0.12 \Rightarrow \exp(-Pe) = 2.4E^{-4}$ kan försummas

$Pe^{-1} = 0.88 \Rightarrow$ insättning i

$$\frac{D_{ea}}{vL} = \frac{0.2111}{2} + \left(\frac{D_{ea}}{vL}\right)^2\left(1 - \exp\left(-\frac{vL}{D_{ea}}\right)\right) \Rightarrow$$

$$\frac{D_{ea}}{vL} = 0.12$$

Ur diagram fås $\frac{C_A}{C_{Af}} = 1 - x = 0.02$

$x = \underline{\underline{0.98}}$

2, Tankseriemodellen

$N = \frac{\tau^2}{\sigma^2} = 4.74$

$\frac{C_A}{C_{Af}} = f(k\tau C_{Af}, N)$

Ur diagram fås $\frac{C_A}{C_{Af}} = 1 - x = 0.02$

$x = \underline{\underline{0.98}}$

3, Ideal tubreaktor

$\langle t \rangle = \frac{L}{v} = \frac{V}{q}$

$\frac{dV}{q} = dt = -\frac{dC_A}{kC_A^2} \Rightarrow t = \frac{1}{k}\left(\frac{1}{C_A} - \frac{1}{C_{Af}}\right)$

$x = 1 - \frac{C_A}{C_{Af}} = 1 - \frac{1}{1 + ktC_{Af}} = \underline{\underline{0.99}}$

3.7} $Pe_a = \frac{u_0 d_p}{D_{ea}} = 2 \Rightarrow Pe = \frac{u_0 L}{D_{ea}} = 20$

$$\Psi_L = \frac{4q\exp(Pe/2)}{(1+q)^2\exp(\frac{Pe}{2}q_-) - (1-q)^2\exp(-\frac{Pe}{2}q_-)}$$

$q = \sqrt{1+4D_A/Pe}$ ej flöde

$D_A = k_c\tau = k_c \frac{W}{q} = 4.9 \Rightarrow q = 1.407$

($q \sim$ flöde)

$\Psi_L = \frac{C_A}{C_{Af}} = 0.017 = 1.7\%$

Idealt

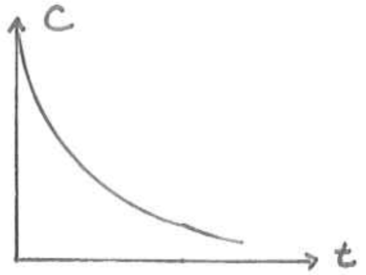
$qC_A - q(C_A + dC_A) - k_c C_A dW$

$\frac{dC_A}{dW} = -\frac{k_c C_A}{q} \Rightarrow \ln\left(\frac{C_A}{C_{Af}}\right) = -\frac{k_c W}{q}$

$\Rightarrow \frac{C_A}{C_{Af}} = \exp\left(-\frac{k_c W}{q}\right) = 7.4E^{-3} \approx 0.7\%$

3.8)

a)



$\Rightarrow$ tankreaktor

b) $qC_{A0} - qC_A - kC_AV = 0 \Rightarrow$

$$\frac{C_A}{C_{A0}} = \frac{q}{q + kV} = \frac{1}{1 + kt} = 1 - X$$

$$\langle t \rangle = \int t \cdot E(t) = \int \frac{t \cdot C_s}{444.225}$$

t	$t \cdot C_s$
0.1	0.02
0.2	0.034
1	0.15
2	0.25
5	0.35
10	0.2
30	0.03

$\Rightarrow \langle t \rangle = 4.99$

$\Rightarrow 1 - X = 0.57$

$\Rightarrow X = \underline{\underline{0.43}}$

3.9}

a, $\bar{t} = \frac{3}{0.01} = 300 \text{ s}$ $\sigma^2 = 15 s^2$

$$\frac{\sigma^2}{\bar{t}^2} = \frac{2}{Pe} - \frac{2}{Pe^2}(1 - \exp(Pe))$$

Miniräknarens ekvationslösare ger: Pe = 5141

$$Pe = \frac{u \cdot L}{D_A} \Rightarrow D_A = 5.836 E^{-6} \ m^2/s$$

b, $$\Psi_L = \frac{4q\exp(Pe/2)}{(1+q)^2\exp(Pe\,q/2) - (1-q)^2\exp(-Pe\,q/2)}$$

$$q = \sqrt{1 + \frac{4 D_A}{Pe}}$$

$$D_A = \frac{k \cdot L}{u} = 6 \Rightarrow q = 1.001943259$$

$$\Rightarrow \Psi_L = 0.0025 \Rightarrow x = \underline{\underline{0.9975}}$$

3.10) $X = 1 - \Psi_L$

$$\Psi_L = \frac{4q\exp(Pe/2)}{(1+q)^2\exp(Pe\,q/2) - (1-q)^2\exp(-Pe\,q/2)}$$

$$q = \sqrt{1 + 4\frac{Da}{Pe}}$$

$$Da = \frac{kL}{u} = k\tau$$

$$\frac{\sigma^2}{\tau^2} = \frac{2}{Pe} - \frac{2}{Pe^2}(1 - \exp(-Pe))$$

$$\tau = \int t \cdot E(t) = 607.6923$$

$$\sigma^2 = \int (t-\tau)^2 \cdot E(t) = 16863.405$$

$\Rightarrow Pe = 42.77255$

$Da = 3.03846$

$\Rightarrow q = 1.133203691$

$\Rightarrow \Psi_L = 0.0576$

$\Rightarrow X = \underline{\underline{0.9424}}$

3.12) $E(\langle t\rangle) = \frac{1}{2\langle t\rangle}\sqrt{\frac{VL}{\pi D_L}}$ $\quad \langle t\rangle = \tau$

$$\tau = \int t \cdot E(t) = 374.4\ s$$

$$E(\tau) = \frac{C_s(\tau)}{\Delta t \int C_s} = \frac{C_s(\tau)}{120 \cdot 50}$$

$$C_s(360) - C_s(\tau) = \frac{12.5 - 10}{360 - 480}(360 - 374.4)$$

$$\Rightarrow C_s(\tau) = 12.2$$

$$\Rightarrow E(\tau) = \frac{12.2}{120 \cdot 50} = \frac{1}{2\tau}\sqrt{\frac{VL}{\pi D_L}}$$

$$\frac{VL}{D_L} = \pi\left(\frac{2 \cdot 12.2 \cdot \tau}{120 \cdot 50}\right)^2 = \underline{\underline{0.137}}$$

3.15) $F(t) = 0 \quad 0 \leq t \leq 0.4$

$$F(t) = 1 - \exp(-1.25(t-0.4)) \quad t > 0.4$$

$$E(t) = F'(t) = 1.25\exp(-1.25(t-0.4)) \quad t > 0.4$$

$$\overline{X} = \int X(t) \cdot E(t)$$

Molbalans satsreaktor:

$$\frac{dN_A}{dt} = -kC_AV \quad \Rightarrow \quad X = 1 - \exp(-kt)$$

$$\overline{X} = \int_{0.4}^{\infty} (1 - \exp(-kt)) \cdot 1.25\exp(-1.25(t-0.4))\,dt = \underline{\underline{0.557}}$$

Molbalans tubreaktor:

$$q\frac{dX}{dV} = k(1-X) \quad \Rightarrow \quad X = 1 - \exp(-\tau k)$$

(ej t)

$$\tau = \frac{1}{1.25} + 0.4 = 1.2$$

CSTR med 0.4 s fördröjning

$$\Rightarrow \quad X = \underline{\underline{0.617}}$$

3.16) $E(t) = \frac{C_s}{1452}$

$\int E(t) = 0.8 \Rightarrow$ tiden för att 80% av spårämnet har gått igenom processen

Integrera tills du passerat $\int E(t)\,dt = 0.8$

$\Rightarrow t_i = 69.5$

$\langle t \rangle = \tau = \int t \cdot E(t) = 54\,s$

$V = \pi r^2 \cdot L = 0.393\ m^3$ reaktorvolym

$q = \frac{V}{\tau} = 0.0072$

$V = q \cdot t_i = \underline{\underline{0.5}}\ m^3$ bensin

3.18) $E(t) = \frac{C_s}{6300}$

Molbalans Satsreaktor:

$$\frac{dN_A}{dt} = -kC_AV \Rightarrow \frac{dX}{dt} = -k$$

$$\Rightarrow X = 1 - \exp(-kt)$$

$$0.8 = \int (1 - \exp(-kt)) \cdot E(t)$$

"Trial and error". Testa k tills ekvationen är uppfylld

$$\Rightarrow k = \underline{\underline{0.027}}\ s^{-1}$$

3.19

Molbalans satsreaktor:

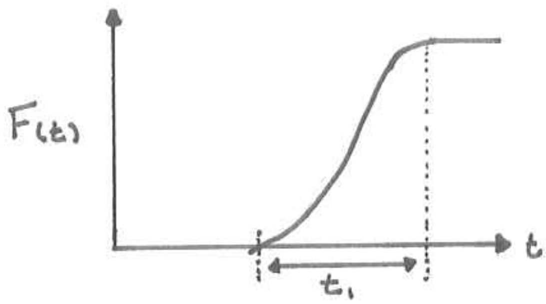
$$\frac{dN_A}{dt} = -kC_A^0 V = -kV \quad \text{"nolte ordningen"}$$

$$\Rightarrow \frac{dC_A}{dt} = -k \quad \Rightarrow \quad C_{A0}\frac{dX}{dt} = k$$

$$\Rightarrow X = \frac{kt}{C_{A0}}$$

$$\bar{X} = \int X \cdot E(t) = \int \frac{kt}{C_{A0}} \cdot \frac{C_S}{255} = \underline{\underline{0.647}}$$

3.20)



t_1 är den tid som rose'n bildas & tas om hand

Antag att rörets diameter samt flödet q är konstant.

Då är dispersionskoefficienten D_A konstant

$$L_2 = \frac{80}{32} L_1 = 2.5\, L_1$$

$$\Rightarrow \tau_2 = 2.5\, \tau_1$$

$$Pe = \frac{u \cdot L}{D_A} \Rightarrow Pe_2 = 2.5\, Pe_1$$

"closed closed"

$$\frac{\sigma_1^2}{\tau_1^2} = \frac{2}{Pe_1} - \frac{2}{Pe_1^2}(1 - \exp(-Pe_1)) \qquad (*)$$

$$\frac{\sigma_2^2}{\tau_2^2} = \frac{2}{Pe_2} - \frac{2}{Pe_2^2}(1 - \exp(-Pe_2))$$

$$\Rightarrow \frac{\sigma_2^2}{6.25\,\tau_1^2} = \frac{2}{2.5\, Pe_1} - \frac{2}{6.25\, Pe_1^2}(1 - \exp(-Pe_2)) \qquad (**)$$

Antag att pluggflödet ej avviker mycket från idealt pluggflöde. ⇒ Pe är stor ⇒

$$6.25\,\frac{\sigma_1^2}{\sigma_2^2} = \frac{2(Pe_1 - 1)}{\frac{2}{2.5}(Pe_1 - 0.4)} = \frac{(*)}{(**)}$$

$(Pe_1 - 1) = (Pe_1 - 0.4)$ om Pe är tillräckligt stor

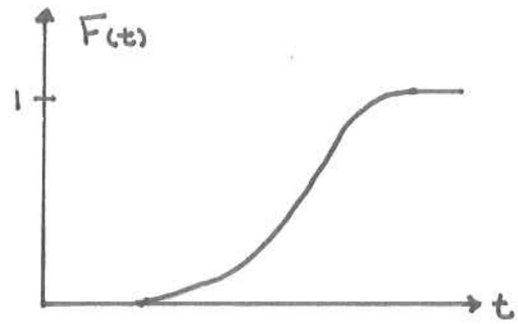
$$\Rightarrow \frac{\sigma_1^2}{\sigma_2^2} = 0.4 \quad \text{och} \quad \frac{\sigma_1}{\sigma_2} = 0.6325$$

σ är propotionell mot antal flaskor b

$$\Rightarrow \frac{\sigma_1}{\sigma_2} = \frac{b_1}{b_2} \quad \Rightarrow \quad b_2 = \frac{8}{0.6325}$$

$\Rightarrow$ $b_2 \approx 12.65$ flaskor rosé

3.21)
$$\frac{\sigma^2}{\tau^2} = \frac{2}{Pe} - \frac{2}{Pe^2}\left(1 - \exp(-Pe)\right)$$



$F(t) = \frac{C_s}{C_{s1}}$

C_s = rågmjölskoncentration

C_{s1} = koncentration av rent rågmjöl

C_s är propotionell mot färgindex I ⇒

$$C_s = K \cdot I \qquad C_{s1} = K \cdot 24 \quad \Rightarrow \quad F(t) = \frac{I}{24}$$

$$\langle t \rangle = \tau = \int_0^1 t \cdot F'(t) = \sum_0^{n-1} \frac{t_i + t_{i+1}}{2} \Delta F_{i+1}$$

$$\tau = \frac{1}{2}\left[(4+10)0.17 + (10+12)0.12 + (12+16)0.29 + (16+24)0.3 + (24+36)0.12\right]$$

$$\tau = 16.17$$

$$\langle t^2 \rangle = \int_0^1 t^2 \cdot F'(t) = \sum_0^{n-1} \frac{t_i^2 + t_{i+1}^2}{2} \Delta F_{i+1}$$

$$\langle t^2 \rangle = \frac{1}{2}\left[(16+100)0.17 + (100+144)0.12 + (144+256)0.29 + (256+576)0.3 + (576+1296)0.12\right]$$

$$\langle t^2 \rangle = 319.62$$

$$\sigma^2 = 319.62 - 16.17^2 = 58.15$$

$$\frac{\sigma^2}{\tau^2} = 0{,}222 = \frac{2}{Pe} - \frac{2}{Pe^2}(1 - \exp(-Pe))$$

$$\Rightarrow Pe = 7.8638$$

$$\Rightarrow D_{ea} = 0.127 \cdot u \cdot L$$

$$u = \frac{L}{\tau}$$

$$\Rightarrow D_{ea} = \underline{\underline{7.85\,E^{-3}}}\ m^2/s$$

$$q = \frac{V}{\tau} = 3.09\,E^{-3}\ m^3/s$$

3.22) Mängd utsläppt PCB: $m = q \int C(t)\,dt$ kg

$$q = \frac{V}{\tau} = \frac{\pi r^2 \cdot L}{\tau}$$

Hur PCB varierar fås ur diagrammet:

$$C(t) - 0.005 = \frac{0.005}{12-36}(t-12) \Rightarrow C(t) = 0.005\left(1.5 - \frac{t}{24}\right)$$

$$\int C(t)\,dt = 0.005\left[1.5t - \frac{t^2}{48}\right]_{12}^{36} = 0.06$$

$$\int t \cdot C(t) = 1.2$$

$$\langle t \rangle = \tau = \frac{1.2}{0.06} = 20 \text{ timmar}$$

$$\Rightarrow m = 0.94 \text{ kg}$$

4.2) $A \rightleftharpoons R$ $\quad r = k_1 C_A - k_2 C_R$

a) isoterm tank: $T = 50°C$

$$qC_{A0} - qC_{A0}(1-X) - (k_1 C_{A0}(1-X) - k_2 C_{A0}(1-X))V = 0$$

$$V = \frac{qX}{k_1(1-X) - k_2 X}$$

$k_1 = 0.4172$

$k_2 = 0.0147$ $\Rightarrow$ $V = \underline{\underline{11.16 m^3}}$

isotermt $\Rightarrow$ $Q_{kyl} = X \cdot \Delta H F_{A0} = \underline{\underline{60.2}}$ MJ/min

b) adiabatisk tank

samma volym som i a, $V = \underline{\underline{11.16}} m^3$

$$q \rho C_p (T - T_f) = F_{A0} X \Delta H \Rightarrow$$

$$T_f = T - \frac{F_{A0} X \Delta H}{q \rho C_p} = -10.25°C$$

c, isoterm tub $T = 50°C$

$$q\int_0^x \frac{dX}{k_1(1-X)-k_2X} = \int_0^V dV \Rightarrow$$

$$V = \underline{\underline{4.08\ m^3}}$$

Q_{KYL} är samma som i a, $= 60.2\ MJ/min$

d, adiabatisk tub

$$V = q\int \frac{dX}{k_1(1-X)-k_2X}$$

$$q\rho C_p(T-T_r) - q\rho C_p(T_{ut}-T_r) + qC_{Af}(X_{ut}-X)(-\Delta H) = 0$$

$$\Rightarrow T = T_{ut} - \frac{C_{Af}(X_{ut}-X)(-\Delta H)}{\rho C_p}$$

X	T(x)	dV(x)
0	263	148.7
0.1	270.5	89
0.2	278	55.8
0.3	285.5	36.7
0.4	293.1	25.3
0.5	300.6	18.5
0.6	308.1	14.5
0.7	315.7	12.7
0.8	323.2	13.8

$$V = q\sum dV_i + \frac{dV(x_i)+dV(x_{i+1})}{2}\cdot\Delta X$$

$$V = \underline{\underline{33.4\ m^3}}$$

4.5)

$$\underset{A}{CO_2} + \underset{B}{3H_2} \rightleftharpoons \underset{C}{CH_3OH} + \underset{D}{H_2O}$$

$$K_p = \frac{P_C P_D}{P_A P_B^3} = \exp\left(-18.2 + \frac{25259}{T}\right)$$

$$K_p = \frac{\frac{F_C}{F_T}P \cdot \frac{F_D}{F_T}P}{\frac{F_A}{F_T}P \cdot \left(\frac{F_B}{F_T}\right)^3 P^3} = \frac{F_C \cdot F_D \cdot F_T^2}{F_A \cdot F_B^3 \cdot P^2}$$

	IN	UT
A	1	$1-x$
B	3	$3-3x$
C	0	x
D	0	x
N_2	10	10
	14	$14-2x = F_T$

$$\Rightarrow K_p = \frac{x^2(14-2x)^2}{(1-x)(3-3x)^3 P^2}$$

$$\Rightarrow T = \frac{25259}{\ln\left(\frac{x^2(14-2x)^2}{(1-x)(3-3x)^3 P^2}\right) + 18.2} \qquad (*)$$

Värmebalans: In − ut + reagerat = 0 $\quad T_r = T_0$

$$\left((1-x)C_{pA} + (3-3x)C_{pB} + xC_{pC} + xC_{pD} + 10C_{pN_2}\right)\Delta T = x \cdot \Delta H$$

$$\Rightarrow T_{ut} = 500 + \frac{210'000\,x}{480-45x} \qquad (**)$$

"plotta (*) och (**) och beräkna skärningen

⇒ $X = \underline{\underline{0.923}}$ $T = \underline{\underline{942}}\,°C$

4.6) $A \rightleftharpoons B$ $\qquad k = \exp\left(-\frac{E_A}{RT}\right) = \exp\left(-\frac{\Delta H}{RT} + \frac{\Delta S}{R}\right)$

$$\Delta H = -250.8\,E^3 + 167.2\,E^3 = -83'600$$

$K = E^5$ då $T = 25°C$

$$\Delta S = \ln(E^5)R + \frac{\Delta H}{T} = -184.677$$

$$C_A = \frac{C_B}{K} \Rightarrow C_{A0}(1-X) = \frac{C_{A0}X}{K} \Rightarrow X = \frac{K}{1+K}$$

$$\Rightarrow \ln\left(\frac{X}{1-X}\right) + \frac{184.677}{R} = \frac{83600}{RT}$$

$$\Rightarrow T = \frac{83600}{R\ln\left(\frac{X}{1-X}\right) + 184.677} \quad (*)$$

Värmebalans: In - ut + reagerat = 0

$$C_{PA}(300-298) - C_P(1-X)(T-300) - C_P X(T-300) + X(-\Delta H) = 0$$

$$\Rightarrow T = \frac{X \cdot \Delta H}{C_P} + 300 \quad (**)$$

"Plotta (*) och (**) och beräkna skärningspunkten

$X = \underline{0.4}$ $\qquad T = \underline{461}\,°C$

4.7) $A \rightleftarrows 2B$

$$K_P = \exp\left(\frac{\Delta H - T\Delta S}{RT}\right) = \frac{P_B^2}{P_A}$$

$T = 127\,^\circ C \Rightarrow K_P = 25E^3 \Rightarrow \Delta S = 7.73\ J/_{mol\,K}$ konstant!

$$\frac{P_B^2}{P_A} = \frac{y_B^2 P^2}{y_A P} = \frac{\left(\frac{F_B}{F_T}\right)^2 \cdot P}{\frac{F_A}{F_T}} = \frac{F_B^2 P}{F_A F_T}$$

	In	ut
A	F_{A0}	$F_{A0}(1-X)$
B	0	$2F_{A0}X$
		$F_T = F_{A0}(1+X)$

$$K_P = \frac{(2F_{A0}X)^2 \cdot P}{F_{A0}(1-X)\,F_{A0}(1+X)}$$

$$\Rightarrow \frac{4X^2 P}{(1-X)(1+X)} = \exp\Big(\overbrace{\frac{\Delta H - T\Delta S}{-RT}}^{\alpha}\Big) \quad (*)$$

$$\Rightarrow (*)\quad X = \frac{R \cdot T \cdot \exp(\alpha)}{4P + RT\exp(\alpha)}$$ jämviktskurva

Driftlinje: $T_r = T_{in} \Rightarrow Q_{in} = 0$

$$(F_{A0}(1-X)C_{PA} + 2F_{A0}XC_{PB})(T_{ut} - T_{in}) = F_{A0}X(-\Delta H)$$

$$\Rightarrow \quad X = \frac{(T - T_{in})C_{PA}}{(-\Delta H) + (C_{PA} + 2C_{PB})(T - T_{in})}$$

Driftlinjen skär jämviktskurvan vid $X = \underline{\underline{0.326}}$ $T = \underline{\underline{655}}\ K$

4.a)

$$CO + 2H_2 \rightleftharpoons CH_3OH$$
A B C

$$K_p = \frac{P_C}{P_A P_B^2} = \frac{\frac{F_C}{F_T}P}{\frac{F_A}{F_T}P \cdot \frac{F_B^2}{F_T^2}P^2} = \frac{F_C F_T^2}{F_A F_B^2 P} = 1.29E^{-13} \cdot 10^{5304/T}$$

	In	ut
A	F_A	$F_A(1-X)$
B	$1.5F_A$	$1.5F_A - 2XF_A$
C	0	F_AX
I	$3F_A$	$3F_A$
	$5.5F_A$	$5.5F_A - 2XF_A$

$$K_p = \frac{F_AX(5.5F_A - 2XF_A)^2}{4F_A(1-X)(1.5F_A - 2XF_A)^2 P^2}$$

$$\Rightarrow T = \frac{5304}{13 + \log\left(\frac{(5.5-2X)^2X}{(1-X)(1.5-2X)^2P^2 1.29}\right)}$$ jämviktskurva!

Värmebalans: $T_r = T_{ut}$

$$(F_A C_{pA} + 1.5F_A C_{pB} + 3F_A C_{pI})(T - T_0) = -XF_A\Delta H$$

$$\Rightarrow T = T_0 - \frac{X\Delta H}{C_{pA} + 1.5C_{pB} + 3C_{pI}}$$ Driftlinje

4.10} $SO_2 + \frac{1}{2} O_2 \rightleftharpoons SO_3$ $P = 1.3$ bar

A B C

$$K_P = \frac{y_C P}{y_A P (y_B P)^{0.5}} = \frac{F_C F_T^{0.5}}{F_A \cdot F_B^{0.5} P^{0.5}} = \exp\left(\frac{11595}{T} - 11\right)$$

	In	ut
A	F_A	$F_A(1-X)$
B	F_B	$\frac{0.3}{0.5} F_A - \frac{1}{2} X F_A$
C	0	$F_A X$
I	F_I	$\frac{0.2}{0.5} F_A$
		$F_T = 2F_A - 0.5 X F_A$

$$\Rightarrow K = \frac{X(2-0.5X)^{0.5}}{(1-X)(3/5 - \frac{1}{2}X)^{0.5} P^{0.5}} = \exp\left(\frac{11595}{T} - 11\right)$$

$$\Rightarrow T = \frac{1}{\ln\left(\frac{X}{1-X}\left(\frac{2 - \frac{1}{2}X}{3/5 - \frac{1}{2}X}\right)^{0.5} \cdot P^{-0.5} + 11\right)}$$

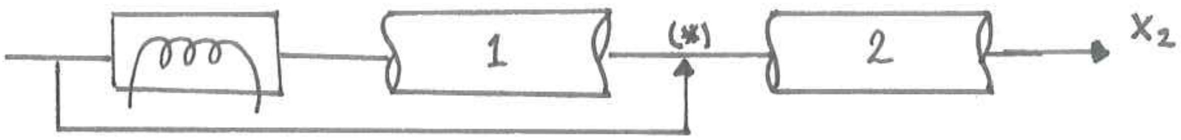
Driftlinje : $T_{ut} = T_r \Rightarrow (F_A C_{PA} + 3/5 F_A C_{PB} + 2/5 F_A C_{PI}) \Delta T = X F_A \Delta H$

$$\Rightarrow T_0 = T - \frac{X \Delta H}{C_{PA} + 3/5 C_{PB} + 2/5 C_{PI}}$$

$X = 0.5 \Rightarrow T = 993.3$ K från jämviktskurva

$\Rightarrow T_0 = \underline{\underline{453.4}}$ K

4.11) $A \rightleftharpoons R$ $\quad F/F_1 = 2 \quad F_A/F_T = 0.04$



$$(0.04 F_T C_p + F_T C_p)(T_{ut} - T_{in}) = -0.04 F_T \Delta X \Delta H$$

$$\Rightarrow T_{ut} = T_{in} + \frac{(X_1 - X_{1f}) \cdot 0.04 \Delta H}{(0.04 + 1) C_p} = 663.15 + 86.53846 \Delta X$$

driftlinje

Rita in jämviktskurvan i miniräknaren & se var den skär driftlinjen.

$$\Rightarrow \quad X_1 = \underline{\underline{0.64}} \quad T_1 = \underline{\underline{720\ K}}$$

$$(*): 0.04 F_T (1 - X_1) + F_T + 2 \cdot 0.04 F_T + F_T X_1 + F_T = F_T$$

$$0.04 F_1 X_1 + 2F_1 \cdot 0.04 X_0 \,(\to 0) = 3 \cdot 0.04 F_1 \cdot X_{2f} \quad \Rightarrow \quad X_{2f} = \frac{X_1}{3}$$

$$F_1 C_p (T_1 - T_f) + 2 F_1 C_p (T_f - T_f) = 3F (T_{2f} - T_f) C_p$$

$$\Rightarrow T_{2f} = \frac{T_1 - T_f}{3} + T_f = 522.1\ K$$

$$(3 \cdot 0.04 F_T X_{2f} + F_T)(T_2 - T_{2f}) = X_2 \Delta H \cdot 0.04 F_T X_{2f}$$

$$T = T_{2f} + 86.53846 (X_2 - X_{2f}) + \text{jämviktskurva} \Rightarrow$$

$$X_2 = \underline{\underline{0.93}} \quad T_2 = \underline{\underline{582}}\ K$$

4.12) $SO_2 + \frac{1}{2} O_2 \rightleftharpoons SO_3$
(A, B, C)

	In	ut
A	F_A	$F_A(1-x)$
B	$\frac{3}{4} F_A$	$\frac{3}{4} F_A - \frac{x}{2} F_A$
C	0	$F_A x$
I	$10.75 F_A$	$10.75 F_A$

$F_T = 12.5 - x/2$

Värmebalans: $T_r = T_{in}$ ⇒ intermen stryks

$$F_A (C_{PA} + \tfrac{3}{4} C_{PB} - \tfrac{x}{2} C_{PB} + x C_{PC} + 10.75 C_{PI})(T - T_{in}) = F_A X \Delta H$$

$$T = \frac{X \Delta H}{409 + 59.5X} + T_{in}$$ + jämviktskurva ⇒

$T = 869.35\ K$

$X = 0.7766$

$$A = \frac{1-X}{F_T} = 0.018$$

$$B = \frac{3/4 - X/2}{F_T} = 0.03$$

$$C = \frac{X}{F_T} = 0.064$$

$$I = 1 - A - B - C = 0.888$$

5.3) Yoshida:

$$\frac{k_{GA} \cdot P_{fA}}{G_m} Sc^{2/3} = 0.84\, Re^{-0.51}$$

$$G_m = \frac{G}{M} = \frac{v \rho}{M} = 2.5$$

$$Sc = 0.75$$

$$Re = \frac{G}{\mu S v \phi} = \frac{0.1\, d_p}{\mu 6 (1-\varepsilon) \phi} = 9.259$$

$$k_{GA} = \frac{0.84\, Re^{-0.51}\, G_m}{Sc^{2/3}\, P_{fA}} \approx \underline{\underline{8.2\, E^{-6}}}$$

5.4)

$$j_D = \frac{k_G P_{fA}}{G_m} Sc^{2/3} = 0.57\, Re^{-0.41}$$

$$k_G = \frac{0.57\, Re^{-0.41}}{P_{fA}} Sc^{-2/3} G_m$$

$$Re = \frac{G}{S_v \mu \phi} = \frac{G\, d_p}{6(1-\varepsilon)\mu} = 55$$

$$G_m = \frac{G}{\langle M \rangle} = 62.0462$$

$$\Rightarrow \quad k_G = 1.1\,E^{-6}\ \text{mol/s m}^2\,\text{Pa}$$

0 snabb reaktion

$$r = k_G (P_{oo} - P_s)$$

$$r' = r\, a_c = r \cdot \frac{6}{d_p \rho_p} = r \cdot \frac{6(1-\varepsilon)}{d_p \rho_b} = 0.34\ \text{mol/s kg kat}$$

5.5} Massbalans tubreaktor:

$$G_m A \frac{dP}{P_{TOT}} = r\,dW$$

Masstransport i porös bädd

$$r = -S_m k_G (P_b - P_s)\phi$$

$$\phi = 1 \qquad P_s = 12\ Pa$$

$$\Rightarrow \frac{-G_m A}{S_m P_{TOT} k_G} \int_0^{0.9P_s} \frac{dP_b}{P_s - P_b} = \int_0^W dW$$

$$\Rightarrow W = \frac{-G_m A}{S_m P_{TOT} k_G} \ln(0.1)$$

$$k_G = j_D \frac{G_m}{P_{TOT}} Sc^{-2/3} = 1.8\,Re^{-0.5} \frac{G}{M P_{TOT}} \cdot Sc^{-2/3} = 1.2268\,E^{-5}$$

$$\Rightarrow W = 0.029 = \underline{\underline{29}}\ g$$

5.6)
$$N_A = \frac{r}{a_c} = \frac{k C_A}{a_c} = \frac{kP}{RT} \cdot \frac{d_p \rho_p}{6}$$

$$q = h \Delta T = N_A(-\Delta H_f)$$

$$\Delta T = \frac{N_A(-\Delta H_f)}{h\, a_c} = \frac{kP}{RT} \cdot \frac{d_p \rho_p}{6} \cdot \frac{(-\Delta H_f)}{h} = \underline{\underline{95}}\,^\circ C$$

5.7) $A \rightarrow B$ $N_A = k_{cA}(C_\infty - C_s)$, $C_s \rightarrow 0$ snabb reaktion

$$j_D = \frac{Sh}{Sc^{1/3} Re} = 0{,}57\, Re^{-0{,}41}$$

$$Re = \frac{G}{S_v \mu \phi}$$

$$G = u \cdot \rho \qquad S_v = \frac{6}{d_p}(1-\varepsilon) \Rightarrow Re = 139$$

$$Sh = \frac{k_{cA} d_p}{D_A} = 0{,}57\, Re^{0{,}59}\, Sc^{1/3}$$

$$\Rightarrow k_{cA} = 6{,}5\,E^{-5}\ m/s$$

$$N_A = k_{cA} C_\infty \sim mol/m^2 s$$

$V_B (1-\varepsilon) S_p$ = total partikelyta i bädden

$$N_A V_B (1-\varepsilon) S_p = 94\ mol/s$$

5.8) Molbalans tubreaktor

$$q\, dC_{Ab} = -r\, dV$$

Strömning i porös bädd

$$r = S_v k_c (C_{Ab} - C_{As})\, \phi$$

$C_{As} \to 0$ snabb reaktion

$$S_v = \frac{6}{d_p}(1-\varepsilon)$$

$$\Rightarrow q\, dC_{Ab} = -S_v k_c C_{Ab}\, dV$$

$$k_c = \frac{D}{d_p} \cdot 1.8 \left(\frac{u\, d_p}{\nu}\right)^{1/2} \left(\frac{\nu}{D}\right)^{1/3} \quad (*)$$

$$u = q/A = q \frac{4}{d^2 \pi} \quad m/s$$

$$V = H \cdot A = H \cdot \frac{\pi d^2}{4} \quad m^3$$

$$-q \int_{C_{A1}}^{C_{A2}} \frac{dC_{Ab}}{S_v k_c C_{Ab}} = \int_0^V dV$$

$$\Rightarrow \frac{-q}{S_v k_c} \ln\left(\frac{C_{A2}}{C_{A1}}\right) = H \frac{\pi d^2}{4} \quad (**)$$

(*) i (**) $\Rightarrow$

$$\frac{-q}{S_v}\frac{d_p}{1.8D}\left(\frac{q\,4\,d_p}{d^2\pi\nu}\right)^{-1/2}\left(\frac{\nu}{D}\right)^{-1/3}\ln\left(\frac{C_{A2}}{C_{A1}}\right) = H\pi\frac{d^2}{4}$$

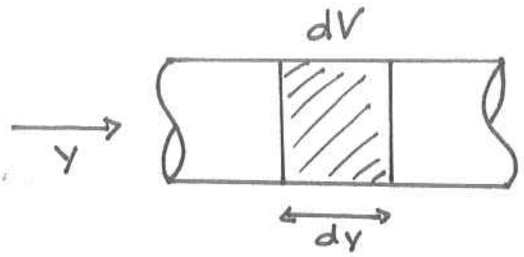
$$\Rightarrow H\cdot d = -\frac{q}{S_v}\frac{d_p}{1.8D}\left(\frac{q\,4\,d_p}{\pi\nu}\right)^{-1/2}\left(\frac{\nu}{D}\right)^{-1/3}\ln\left(\frac{C_{A2}}{C_{A1}}\right)\frac{4}{\pi}$$

$$\Rightarrow H\cdot d = \underline{\underline{0.102}}\ m^2$$

5.9) Massbalans tubreaktor

$$q \, dC_{Ab} = r \, dV$$

$$v \, dC_{Ab} = r \, dy$$



Strömning genom porös bädd

$$r = -S_v k_c (C_{Ab} - C_{As})$$

$$\Rightarrow \quad v \, dC_{Ab} = -S_v k_c (C_{Ab} - C_{As}) \, dy \quad \Rightarrow$$

$$\int_0^{C_{Ab}} \frac{dC_{Ab}}{C_{Ab} - C_{As}} = -S_v \frac{k_c}{v} \int_0^L dy \quad \Rightarrow$$

$$S_v L = \frac{\ln\left(1 - \frac{C_{Ab}}{C_{As}}\right)}{\left(\frac{k_c}{v}\right)} \qquad \frac{C_{Ab}}{C_{As}} = 0.9 \text{ för luft}$$

$$j_D = \frac{Sh}{Re \, Sc^{1/3}} = \frac{k_c}{v} Sc^{2/3} = \frac{k_c}{v} \left(\frac{\nu}{D}\right)^{2/3}$$

$$\left(\frac{k_c}{v}\right)_{luft} Sc_{luft}^{2/3} = \left(\frac{k_c}{v}\right)_{vatten} Sc_{vatten}^{2/3} \quad \text{för samma } Re$$

$$\Rightarrow \frac{\left(\frac{k_c}{v}\right)_{vatten}}{\left(\frac{k_c}{v}\right)_{luft}} = 0.01 \qquad \frac{k_c}{v} = \alpha$$

$$\ln\left(1 - \frac{C_{Ab}}{C_{AS}}\right) = \underbrace{\frac{\alpha_{vatten}}{\alpha_{luft}}}_{0.01} \cdot \ln(0.1) = 0.01$$

$$\Rightarrow \frac{C_{Ab}}{C_{AS}} = 1 - \exp\left(0.01 \cdot \ln(0.1)\right) = 0.02276$$

$$\Rightarrow \frac{C_{Ab}}{C_{AS}} \approx \underline{\underline{2.28\,\%}}$$

5.10) $SO_2 + \frac{1}{2} O_2 \rightarrow SO_3$

$N_{A1} = k_L a (C^* - C_b)$ Transport av O_2 från bubbla genom filmen till bulken.

$N_{A2} = k_c a_s (C_b - C_s)\phi$ Transport av O_2 från bubbla genom filmen till katalysatorns yta

C^* - syrets löslighet mol/m³ reaktor

C_b - syrets bulkkoncentration mol/m³

C_s - syrets ytkoncentration mol/m³

a - våtskans yta/ reaktorvolym $m^2/m^3 = m^{-1}$

a_s - katalysatoryta/ reaktorvolym $m^2/m^3 = m^{-1}$

ϕ - formfaktor = 1 för sfäriska partiklar

$$C^* - C_s = \frac{N_1}{k_L a} + \frac{N_2}{k_c a_s}$$

$r = k C_s a_s$ reaktionshastighet $\Rightarrow$

$$C^* - \frac{r}{k a_s} = \frac{N_1}{k_L a} + \frac{N_2}{k_c a_s}$$

Vid stationära betingelser är :

$N_1 = N_2 = r \quad \Rightarrow$

$$\frac{c^*}{N_1} = \frac{1}{k_c a_s} + \frac{1}{k_L a} + \frac{1}{k\, a_s} \Rightarrow$$

$$N_1^{-1} = \frac{1}{k_L a c^*} + \frac{1}{a_s c^*}\left(\frac{1}{k} + \frac{1}{k_c}\right) \Rightarrow$$

$N_1^{-1} = f(a_s)$ Rät linje där skärningen ger k_L

gas - vätska

$$\left.\begin{aligned} a &= 4\pi\left(\frac{d_g}{2}\right)^2 \cdot n_g \\ n_g &= \frac{4}{3}\pi\left(\frac{d_g}{2}\right)^3 V_g \end{aligned}\right\} \quad a = \frac{6 V_g}{d_g}$$

d_g - gasbubblans diameter m

V_g - volym gas/reaktorvolym m^3/m^3

n_g - antal gasbubblor/reaktorvolym

vätska - katalysator

$$\left.\begin{aligned} a_s &= 4\pi\left(\frac{d_p}{2}\right)^2 n_p \\ n_p &= \frac{4}{3}\pi\left(\frac{d_p}{2}\right)^3 \rho_p = m_p \end{aligned}\right\} \quad a_s = \frac{6 m_p}{d_p \rho_p}$$

d_p - partikelns diameter m

n_p - antal partiklar/reaktorvolym

ρ_p - partiklarnas densitet kg/m^3

m_p - katalysatormassa/reaktorvolym kg/m^3

$$\underbrace{N_1^{-1}}_{y} = \underbrace{\frac{d_g}{k_L C^* 6 V_g}}_{m} + \underbrace{\frac{1}{m_p} \cdot \frac{\rho_p d_p}{6 C^*} \left(\frac{1}{k} + \frac{1}{k_c} \right)}_{kx}$$

$$\Rightarrow \quad y = kx + m$$

N_1	y	m_p
$8.4 \; 10^{-3}$	119	13.1
$4.22 \; 10^{-3}$	237	5.6
$1.78 \; 10^{-3}$	562	2.22

Minsta kvadratmetoden $\Rightarrow$ $m = 27.195$

$$k_L = \frac{d_g}{m C^* 6 V_g} = \underline{\underline{1.12 \; 10^{-3}}} \; m/s$$

$$k_L a = \frac{1}{m C^*} = \underline{\underline{0.165}} \; s^{-1}$$

6.3) Snabb pordiffusion $\Rightarrow \eta = 1$

$r_0 = k C_{AS}$ reaktionshastighet

$r = \eta k C_{AS}$ observerad reaktionshastighet

$$\phi = \frac{d_P}{2}\sqrt{\frac{k}{D_e}}$$

$$\frac{\phi_2}{\phi_1} = \frac{d_{P2}}{d_{P1}} = \frac{0.25}{1.75} = \frac{1}{7}$$

$$\frac{\eta_1}{\eta_2} = \frac{r_1}{r_2} = \frac{0.035}{0.07} = \frac{1}{2}$$

Diagram $\Rightarrow \phi_1 = 5$

$$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi}\right)$$

$$\phi = 5 \Rightarrow \tanh(\phi) \approx 1 \Rightarrow \eta = 0.48$$

$$r_0 = \frac{r_1}{\eta} = k C_{AS} = \frac{0.035}{0.48} = \underline{\underline{0.0729}} \text{ kmol/s kg katalysator}$$

6.5) Första ordningens reaktion med avseende på A

a) $N_A = k_c \cdot C_{Ab} \cdot \phi = 1.66 \text{ mol/sm}^2$

$r \cdot \frac{1}{S_p} = r \cdot \frac{d_p}{6} = 0.01 \text{ mol/s}$

$\Rightarrow C_{AS} \neq 0$ yttre filmmotstånd ej dominerande

b) Weisz - Prater

$C_{wp} = \eta \phi_1^2 < 1$ då inre motståndet är litet

$C_{wp} = \frac{r^* \rho r_p^2}{D_e C_{AS}}$ (r_p ~ radie) $r^* \sim$ mol/s kg katalysator $\Rightarrow$

$C_{wp} = \frac{r d_p^2}{4 D_e C_{Ab}} = 143$ inre motstånd stort

(C_{Ab} ~ filmtransporten ej begränsande)

c) $q = h_g A \Delta T = r(-\Delta H) V_p \Rightarrow \Delta T = T_s - T_b = 39.6 \text{ K}$

d) $\Delta T = \frac{D_e(-\Delta H)\Delta C}{\lambda_e}$ maximala $\Rightarrow C_A = 0 \Rightarrow$

$\Delta T = 0.1$ ty $C_{AS} \approx C_{Ab}$ enligt b)

6.6) $A \rightarrow R$ första ordningens process

$$\phi = \frac{d_p}{2}\sqrt{\frac{k_n S_A \rho_p C_{AS}^{n-1}}{D_e}}$$

$k_n \sim$ mol/s m² intern yta

$r \sim$ mol/m³ katalysator i vårt fall

$k_n \cdot S_A \cdot \rho \sim$ mol/s m³ katalysator $\Rightarrow$

$$k_n = \frac{k}{S_A \rho} \Rightarrow \phi = \frac{d_p}{2}\sqrt{\frac{k}{D_e}}$$

Weisz-Prater

$C_{WP} = \eta \phi^2 < 1$ då inre motståndet är litet

$$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi}\right) \Rightarrow$$

$$\phi^2 \eta = 3\left(\frac{\phi}{\tanh(\phi)} - 1\right) < 1 \Rightarrow \frac{\phi}{\tanh(\phi)} \leq \frac{4}{3}$$

ekvationslösaren ger $\phi \leq 1.034 = \frac{d_p}{2}\sqrt{\frac{k}{D_e}}$

$$\Rightarrow \frac{d_p}{2} = \underline{\underline{0.01034}}$$

6.7) $r = k_v C_A \sim mol/_{s\,m^3 katalysator}$

$N_A = k_c \Delta C S_p \sim mol/_{s\,m^3 katalysator}$ $\Rightarrow$

$$k_v C_{AS} \eta = -S_p k_c (C_A - C_{AS})\,\phi \qquad \phi = 1 \quad \Rightarrow$$

$$C_{AS} = \frac{S_p k_c C_A}{k_v \eta + S_p k_c} \qquad \text{behöver } \eta \text{ \& } C_A$$

$$k_v \sim \frac{m^3 gas}{s\, m^3 kat} \Rightarrow k_n = \frac{k_v}{S_A \rho} \Rightarrow$$

$$\phi = \frac{d_p}{2}\sqrt{\frac{k_v}{De}} = 3.043$$

$$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi}\right) = 0.6664$$

$$C_A = \frac{F_{A0}(1-x)}{F_{TOT}} \cdot \frac{P}{RT}$$

$$F_{TOT} = q C_{A0}(1-x) + 2 q C_{A0} X = q C_{A0}(1+x) \Rightarrow$$

$$C_A = \frac{1-x}{1+x}\,\frac{P}{RT} = 4.603 \Rightarrow$$

$$C_{AS} = 4.284$$

$$N_A = k_c S_p (C_A - C_{AS}) = 2.2 \cdot 10^{-3} \; mol/_{s\,m^2}$$

6.8) $3A + B \rightarrow C + 2D$

Henrys lag

$P_A = C_{Ab} \cdot He \Rightarrow C_{Ab} = 0.8$ bulkkoncentration vätgas

$3r_B = r_A$ 3 väte reagerar med 1 RNO_2

$k_c a_c (C_{Ab} - C_{As}) \sim r_B \sim mol/s\, kg\, kat$

$3r_B = k_c a_c (C_{Ab} - C_{As})$ transporterat = reagerat

$Sh = \frac{k_c d_p}{D} = 4 \Rightarrow k_c = 5.7 \cdot 10^{-4}\ m/s \Rightarrow$

$C_{As} = C_{Ab} - \frac{3r_B}{k_c a_c} = 0.5533$

$\eta = \frac{r_B}{r} = \frac{r_B}{kC_{As}}$ (1)

$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi}\right)$ antag $\phi > 5 \Rightarrow \tanh(\phi) \approx 1 \Rightarrow$

$\eta \phi^2 = 3(\phi - 1)$ (2)

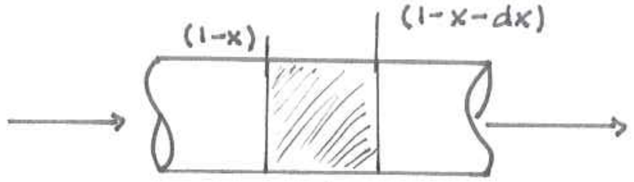
$\phi = \frac{d_p}{2}\sqrt{\frac{k_n S_A \rho}{De}}$ $k_n \sim \frac{k}{S_A} \Rightarrow$

$k = \frac{4\phi^2 De}{d_p^2 \rho_p}$ (3)

(1) & (3) $\Rightarrow \eta = \frac{r_B d_p^2 \rho_p}{4\phi^2 De C_{As}}$

$\eta \phi^2 = \frac{r_B d_p^2 \rho_p}{4 De C_{As}} = 3(\phi - 1) \Rightarrow \phi = 8.2 > 5 \Rightarrow \eta = \underline{\underline{0.32}}$

6.9) $A + B \xrightarrow{H^+} C + D$ $\qquad r = k_v C_A \sim \text{kmol}/_{s\,m^3\,kat}$



$dW = dV(1-\varepsilon)$

Massbalans tubreaktor

$$qC(1-x) - qC(1-x-dx) = r\,dV(1-\varepsilon) \Rightarrow$$

$$\frac{C\,dX}{r} = \frac{dV(1-\varepsilon)}{q} \qquad r = \eta k_v C_s$$

Försumbart filmmotstånd $\Rightarrow C_s = C_b = C(1-x)$

$$\frac{1}{\eta k_v}\int_0^x \frac{dX}{1-x} = \int_0^V \frac{(1-\varepsilon)\,dV}{q} \Rightarrow$$

$$\eta k_v = -q\frac{\ln(1-x)}{V(1-\varepsilon)} = 5{,}07 \cdot 10^{-3}\ m/s$$

$$\eta = \frac{3}{\phi}\left(\frac{1}{\tanh(\phi)} - \frac{1}{\phi}\right) \qquad \phi > 5 \Rightarrow \tanh(\phi) \approx 1 \Rightarrow$$

$$\eta\phi^2 = 3(\phi - 1)$$

$$k_n = \frac{k_v}{S_A \rho} \Rightarrow \qquad \phi = \frac{d_p}{2}\sqrt{\frac{k_v}{D_e}} \Rightarrow$$

$$\eta = \frac{3 D_e 4}{d_p^2 k_v}\left(d_p \sqrt{\frac{k_v}{D_e}} - 1 \right) \Rightarrow$$

$$\eta k_v = \frac{12 D_e}{d_p^2}\left(d_p \sqrt{\frac{k_v}{D_e}} - 1 \right) = 5{,}07 \cdot 10^{-3} \Rightarrow$$

$$k_v = \underline{\underline{0{,}0193}} \ s^{-1}$$

$$\phi = \frac{d_p}{2}\sqrt{\frac{k_v}{D_e}} = 10{,}31 > 5 \quad \text{OK!}$$

6.10) $-r_A = k_v C_A^2$

$$\phi = \frac{d_p}{2}\sqrt{\frac{k_n S_A \rho C_A}{D_e}}$$

$$k_n \sim \frac{k_v}{S_A \rho} \Rightarrow \phi = 50$$

Stor ϕ $\Rightarrow$

$$\eta = \left(\frac{2}{n+1}\right)^{1/2} \frac{6}{d_p}\sqrt{\frac{D_e}{k_v}}\, C_{AS}^{(1-n)/2}$$

$n = 2 \Rightarrow \eta = \underline{\underline{0.049}}$