21/3-18 Föreläsning

Ideala reaktorer

Reaktionshastighet

$aA + bB \rightarrow cC + dD$

stökiometrisk koefficient : $\nu \Rightarrow$

$\nu_A = -a$

$\nu_B = -b$

$\nu_C = c$

$\nu_D = d$

$r = kC_AC_B$

$r_A = \nu_A r = -akC_AC_B$

$r_B = \nu_B r = -bkC_AC_B$

osv.

$r = f(T, C_A, C_B, C_C, C_D)$

aktiveringsenergi

Arrhenius ekv. $k = Ae^{-\frac{E_A}{RT}}$

hastighets konst.

pre-exp faktor

$R = 8{,}314$

$T =$ temp. i K.

$r = kC_A^{\alpha} C_B^{\beta}$, α, β - reaktionsordning

Reversibel reaktion

$r_{tot} = r_{forward} - r_{bakward}$

ex. $NO + \frac{1}{2}O_2 \underset{r_b}{\overset{r_f}{\rightleftharpoons}} NO_2$

$r_{tot} = r_f - r_b$

Ideala reaktorer - MB

In - Ut ± reagerat / bildats = ackumulerat

tank:

steady - state

$$F_{A_0} - F_A + r_A V = 0$$

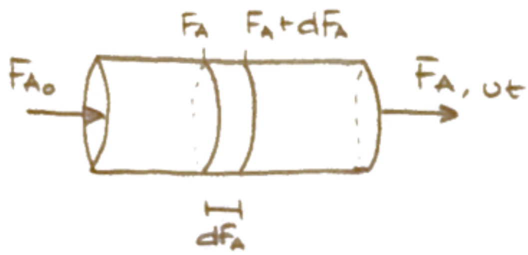
$$\left[\frac{mol}{s}\right] - \left[\frac{mol}{s}\right] + \left[\frac{mol}{s\,m^3}\right]\left[m^3\right]$$

Satsreaktor - batch

Alltid icke-steady-state.

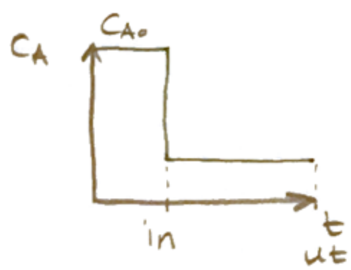
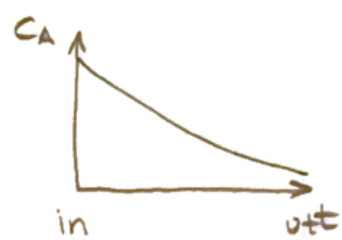
$$0 - 0 + r_A V = \frac{dN_A}{dt}$$

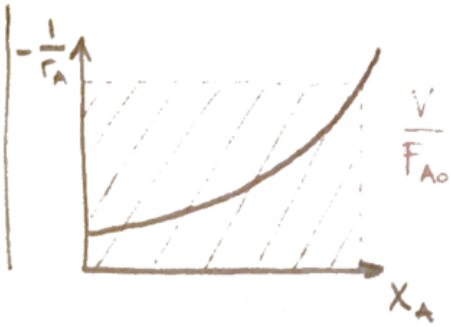
Tubreaktor



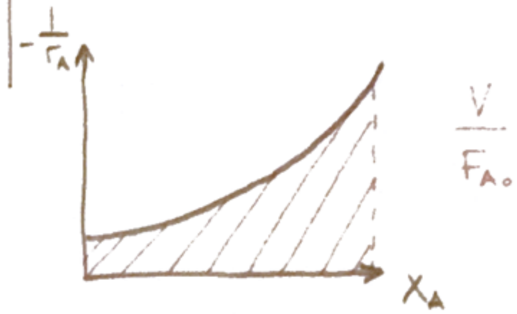
$$F_A - (F_A + dF_A) + r_A dV = 0$$

$$\Rightarrow \frac{dF_A}{dV} = r_A$$

Sats	Tank	Tub
		
		
	$F_{A_0} - F_A + r\,dV = 0$	$dF_A = r_A dV$
	$F_A = F_{A_0}(1 - X_A)$	$dF_A = -F_{A_0} dX_A$
	$F_{A_0} X_A = -r_A V$	$-F_{A_0} dX_A = r_A dV$
	$\frac{V}{F_{A_0}} = X_A \cdot \frac{1}{-r_A}$	$\frac{dX_A}{r_A} = -\frac{dV}{F_{A_0}}$

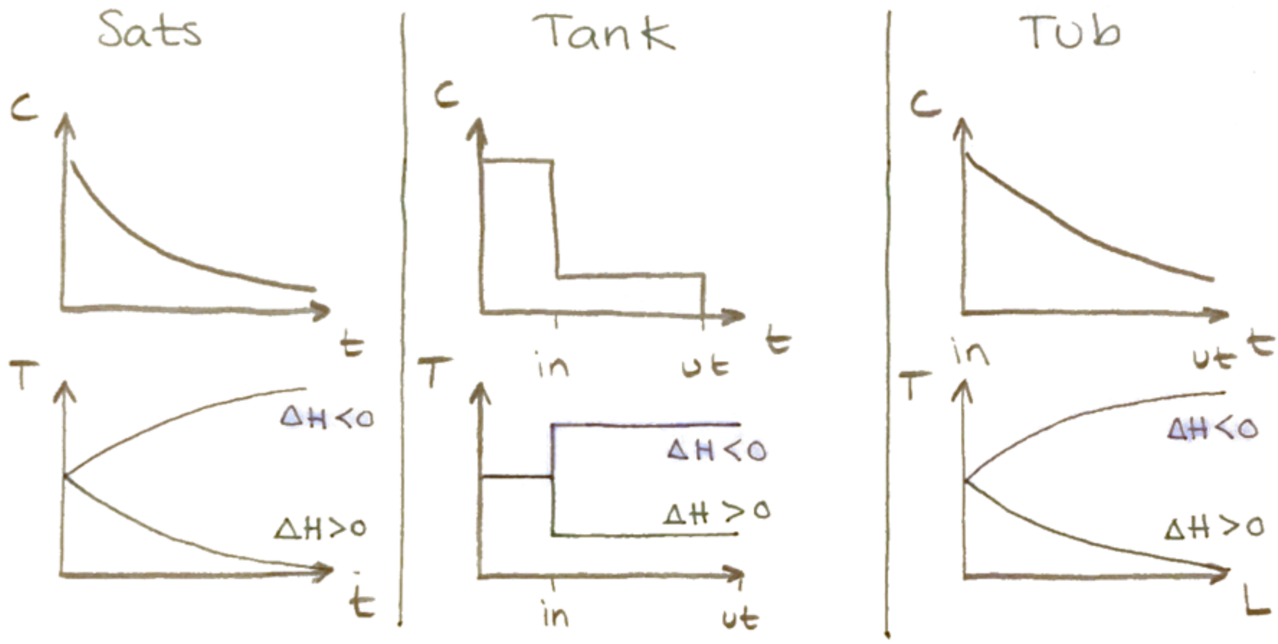


$$\frac{V}{F_{A0}} = \int_0^{X_{ut}} -\frac{dX_A}{r_A}$$



Detta är endast med hänsyn till konc. och med antagandet att allt är perfekt omrört.
Detta fall var även för isoterma fall.

Icke-isotermt:



Endoterm, $\Delta H > 0$: tub eller sats bäst

Exoterm, $\Delta H < 0$: tan <u>kan</u> vara bättre

Första ordn. reaktion, icke-reversibel $r = kC_A$

T ökar $\rightarrow$ ökar k $\rightarrow$ ökar r

Värmebalans

tank

In: $\sum_j F_{j0} \int_{T_{ref}}^{T_0} C_{p_j}\, dT$ [kJ/s]

Ut: $\sum_j F_j \int_{T_{ref}}^{T} C_{p_j}\, dT$ [kJ/s]

reaktion: $rV(-\Delta H_R(T_{ref}))$ [kJ/s]

värme: $\dot{Q}$ [kJ/s]

steady-state: ack = 0

$$T_{ref} = T \Rightarrow \sum_j F_{j0} \int_{T}^{T_{in}} C_{p_j}\, dT + rV(-\Delta H_R(T)) + \dot{Q} = 0$$

om adiabatiskt $\Rightarrow \dot{Q} = 0$

Sats

$$0 - 0 + \dot{Q} + rV(-\Delta H)dt = \sum_j N_j C_{p,j}\, dT$$

Tub

$$Ua_w(T_a - T)\, dz + r(-\Delta H)\, dV = \sum_j F_j C_{p_j}\, dT$$

$\uparrow$
tot. värmeövergångstalet