Tis LV1

Material och energibalanser

Input flow streams → System → output flow streams

$$\{\text{Ackumulation}\} = \{\text{In}\} - \{\text{Ut}\} + \left\{\begin{matrix}\text{Produktion}\\ \text{i systemet}\end{matrix}\right\} - \left\{\begin{matrix}\text{Förbrukning}\\ \text{i system}\end{matrix}\right\}$$

om ingen produktion eller ~~ß~~ förbrukning/arbete:

$$\{\text{Ack.} = \text{In} - \text{Ut}\}$$

Steady-state: In ≡ Ut

~~Massbalans kon~~

① Balans för komponent i med J inflöde och K utflöde:

$$\frac{dN_i}{dt} = \sum_{j=1}^{J} F_i^{j} - \sum_{k=1}^{K} F_i^{K}$$

F_i - molflöde, molär flödes hastighet

N_i - mol av komp. i

→ ~~Detta~~ Detta är utan reaktion!

② Balans för komponent i med J inflöde, K utflöde och M reaktioner

$$\frac{dN_i}{dt} = \sum_{j=1}^{J} F_i^{j} - \sum_{k=1}^{K} F_i^{k} + \sum_{m=1}^{M} \nu_{im} R_m$$

ν_{im} – stökiometrisk koeff. för komp. i i reaktion m

Vid steady state: $F_i^3 + F_i^4 = F_i^1 + F_i^2 + 2R_1 - R_2$

R_m - rate of reaction m

(3) Steady-state balance for atomic species p for I compounds, J inlet streams, K outletstreams:

$$\sum_{k=1}^{K}\sum_{i=1}^{I} \alpha_{ip} F_{ik} = \sum_{j=1}^{J}\sum_{i=1}^{I} \alpha_{ip} F_i^j$$

Fall 1-3 var kontinuerliga flödesprocesser!

"Lösningsgång"

1. Choose a basis for calulations

   Ex. unit of mass

   unit of volume

   unit of time

2. Arrive at the same solution, indep. of basis

Val av dålig bas → onödigt svåra kalkyleringar!

Ex. Propan förbränns i 25% överflöde av luft. Hur många mol luft per sekund behövs för att producera 100 mol avgas per sekund? Lös med 3 olika baser.

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

C_3H_8 (1) → Förbränning → (2) 100 mol/s avgas

25% xs air — O_2, N_2, CO_2, H_2O

Luft: 79 mol% N_2
21 mol% O_2

Basis (1)

$$F^1_{C_3H_8} = 100 \text{ mol/s}$$

$$F^1_{O_2} = (100)(5)(1.25) = 625 \text{ mol/s}$$

$$F^1_{N_2} = 625 \cdot \left(\frac{79}{21}\right) = 2351 \text{ mol/s}$$

$$F^2_{C_3H_8} = F^1_{C_3H_8} - R = 0 \rightarrow R = 100 \text{ mol/s}$$

ty all propan förbränns!

$$F^2_{O_2} = F^1_{O_2} - 5R = 125 \text{ mol/s}$$

$$F^2_{N_2} = F^1_{N_2} = 2351 \text{ mol/s}$$

$$F^2_{CO_2} = \cancel{F^1_{CO_2}} + 3R = 300 \text{ mol/s} \quad (F^1_{CO_2} = 0)$$

$$F^2_{H_2O} = \cancel{F^1_{H_2O}} + 4R = 400 \text{ mol/s} \quad (F^1_{H_2O} = 0)$$

$$F^2_{tot} = 3176 \text{ mol/s}$$

$$F^1_{air} = 2976 \text{ mol/s}$$

vill veta F^{1*}_{air} som ger $F^2_{tot} = 100$ mol/s

vet att $F^1_{air} = 2976$ mol/s → $F^2_{tot} = 3176$ mol/s

Alltså: $$F^{1*}_{air} = 2976\left(\frac{100}{3176}\right) = 937 \text{ mol/s}$$

Basis ②

$$\begin{cases} F^1_{air} = 100 \text{ mol/s} \\ F^1_{O_2} = 21 \text{ mol/s} \\ F^1_{N_2} = 79 \text{ mol/s} \\ F^1_{C_3H_8} = 21/5/1.25 = 3.36 \text{ mol/s} \end{cases}$$

$$\begin{cases} F^2_{C_3H_8} = F^1_{C_3H_8} - R = 0 \rightarrow R = 3.36 \text{ mol/s} \\ F^2_{O_2} = F^1_{O_2} - 5R = 21 - (5 \cdot 3.36) = 4.42 \text{ mol/s} \\ F^2_{N_2} = F^1_{N_2} = 79 \text{ mol/s} \\ F^2_{CO_2} = F^1_{CO_2} + 3R = 10.08 \text{ mol/s} \\ F^2_{H_2O} = F^1_{H_2O} + 4R = 13.44 \text{ mol/s} \end{cases}$$

$$F^2_{tot} = 106.72 \text{ mol/s}$$

$$F^1_{air} = 100 \text{ mol/s}$$

$$\rightarrow F^{1*}_{air} = 100 \cdot \left(\frac{100}{106.72}\right) = 93,7 \text{ mol/s}$$

Basis ③

$F^2_{tot} = 100$ mol/s avgas

$$\left.\begin{array}{l} F^2_{C_3H_8} = F^1_{C_3H_8} - R = 0 \\ F^2_{O_2} = F^1_{O_2} - 5R \\ F^2_{N_2} = F^1_{N_2} \\ F^2_{CO_2} = \cancel{F^1_{CO_2}} + 3R \\ F^2_{H_2O} = \cancel{F^1_{H_2O}} + 4R \end{array}\right\} F^2_{tot} = 100 \text{ mol/s}$$

$$F^2_{N_2} = F^1_{N_2} = \frac{79}{21} F^1_{O_2} = 3.76\, F^1_{O_2}$$

$$F^2_{tot} = 4.76\, F^1_{O_2} + 2R = 100 \text{ mol/s}$$

$$F^1_{O_2} = (5 \cdot 1.25)\, F^1_{C_3H_8}$$

$$F^1_{C_3H_8} = R$$

$$\Rightarrow F^1_{O_2} = 6.25\, R$$

$$F^2_{tot} = 4.76(6.25\, R) + 2R = 100 \text{ mol/s}$$

$$\Rightarrow R = 3.15 \text{ mol/s}$$

$$\left.\begin{aligned} F^1_{O_2} &= 6.25 \cdot R = 19.69 \text{ mol/s} \\ F^1_{N_2} &= 3.76\, F^1_{O_2} = 74.05 \text{ mol/s} \end{aligned}\right\} F^1_{air} = 93.7 \text{ mol/s}$$

Frihetsgrader för materialbalanser

{Frihetsgrader} = {total antal oberoende flödes variabler} − {total antal oberoende balans ekv.} − {total antal specifika flödes variabler} − {total number of supplementary relations}

Frihetsgrader	Problem	Lösningar
>0	under def.	ingal lösn.
0	Definierad	en unik lösn
<0	över bestämd	många

Multi-system balanser

Processer kan innehållar fler sub-system

- Short-cut method
- Tried and true method

Energi balanser

$$\left\{\begin{matrix}\text{Ack av värme} \\ \text{i systemet}\end{matrix}\right\} = \{\text{In}\} - \{\text{ut}\} + \left\{\begin{matrix}\text{Prod av} \\ \text{värme}\end{matrix}\right\} - \left\{\begin{matrix}\text{Förbruk.} \\ \text{av värme}\end{matrix}\right\}$$

Vi tar endast ~~tag~~ hänsyn ~~tg~~ till energi balanser i form av värme balanser.

Dessa görs med entalpi ändringar, ΔH

Värme balans:

Generell, adiabatisk värmebalans

$$\sum N_{i0} \int_{T_{ref}}^{T_0} c_{p_i} \, dT - \sum N_i \int_{T_{ref}}^{T} c_{p_i} \, dT + \sum R_j \left(\underbrace{-\Delta H_{R_j}(T_{ref})}_{\text{reaktionsentalpi vid } T_{ref}}\right) = 0$$

(= 0 tg steady-state)

i - komponent

j - reaktion

Låt $T_{ref} = T_R$:

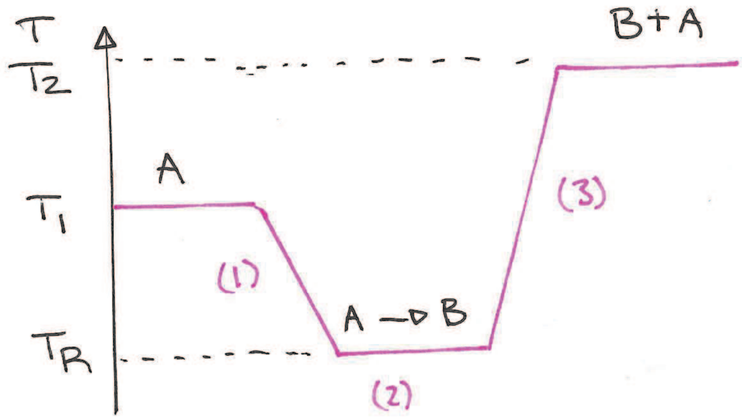
$$N_{A0} \int_{T_R}^{T_1} c_{p_A} \, dT - \left[N_A \int_{T_R}^{T_2} c_{p_A} \, dT + N_B \int_{T_R}^{T_2} c_{p_B} \, dT \right] + R(-\Delta H_R) = 0$$

Processen består av 3 steg

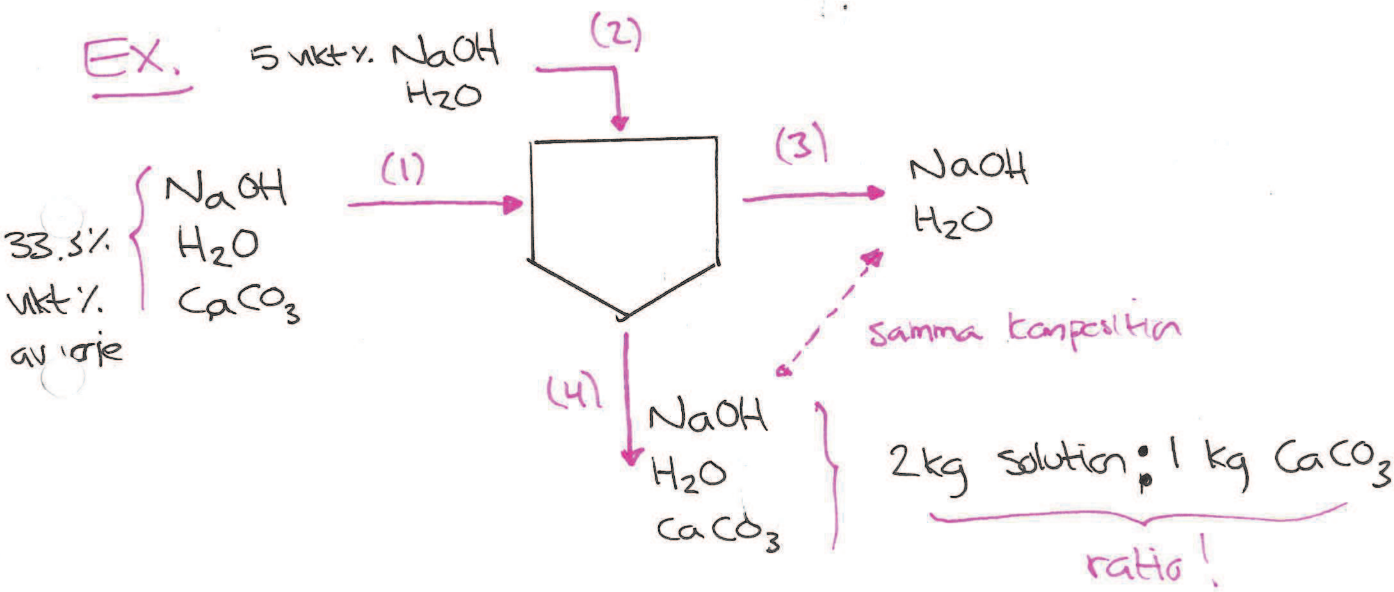
1. kylning av A från $T_1 \rightarrow T_R$
2. reaktion vid T_R
3. värmning av B från $T_R \rightarrow T_2$ (samt återstående A)

Obs! ~~$T_1 < T_R$,~~

$T_1 > T_R$, $T_2 > T_R$, reaktionen pågår vid T_R.



Ex.



Sökt: Om (1) innehåller lika mycket vikt procent av varje komponent, beräkna koncentrationen av (3) och (4)

Basis ① 100 kg/s av (1) och (2)

$$\begin{cases} m_N^1 = 33.3 \text{ kg/s} \\ m_H^1 = m_C^1 = m_N^1 = 33.3 \text{ kg/s} \end{cases}$$

$$\begin{cases} m_N^2 = 5 \text{ kg/s} \\ m_H^2 = 95 \text{ kg/s} \end{cases}$$

$$\frac{m_N^4}{m_H^4} = \frac{m_N^3}{m_H^3}$$ ty samma komposition i (3) och (4)

$$\frac{m_N^4 + m_H^4}{m_C^4} = 2 \Rightarrow m_N^4 + m_H^4 = 2\, m_C^4$$

$CaCO_3$: $m_C^4 + \cancel{m_C^3}_{0} = m_C^1 + \cancel{m_C^2}_{0} \Rightarrow m_C^4 = m_C^1 = 33.3 \text{ kg/s}$

$NaOH$: $m_N^1 + m_N^2 = m_N^3 + m_N^3 = 38.3 \text{ kg/s}$

H_2O: $m_H^1 + m_H^2 = m_H^3 + m_H^4 = 128.3 \text{ kg/s}$

Example

The production of ethylene glycol $(CH_2OH)_2$ occurs by the hydrolysis of CH_2OHCH_2Cl in a $NaHCO_3$ solution according to the reaction formula:

$CH_2OHCH_2Cl + HCO_3^- \rightarrow (CH_2OH)_2 + Cl^- + CO_2$

At 80°C the reaction is second order

$r = k\, C_{CH2OHCH2Cl}\, C_{HCO3}$

Ethylene glycol shall be produced at a rate of 45 kg h^{-1} in a tank reactor operated isothermally at 80°C. Reactants will be supplied from two storage tanks on site, one contains a 15 wt% solution of $NaHCO_3$ and the other a 30 wt% solution of CH_2OHCH_2Cl. The density of both solutions is 1000 kg m^{-3}. The conversion of CH_2OHCH_2Cl over the 38.3 m^3 tank reactor is 95%.

(a) Calculate the rate constant (k) for the reaction.
(b) If the tank reactor were replaced by a tube reactor what would be its required volume?

Molecular weights:

$NaHCO_3$	84 kg $kmol^{-1}$
CH_2OHCH_2Cl	80 kg $kmol^{-1}$
$(CH_2OH)_2$	62 kg $kmol^{-1}$

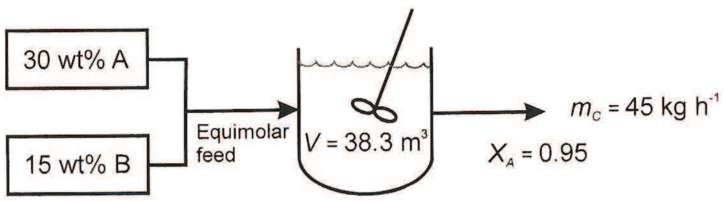
25

Example

$CH_2OHCH_2Cl + HCO_3^- \rightarrow (CH_2OH)_2 + Cl^- + CO_2$

$A + B \rightarrow C + D + E$

$r = k\, C_A\, C_B$



ρ = 1000 kg m^{-1} (density of solutions)
M_A = 80 kg $kmol^{-1}$
M_B = 84 kg $kmol^{-1}$
M_C = 62 kg $kmol^{-1}$

(a) k = ?
(b) V_{tube} = ?

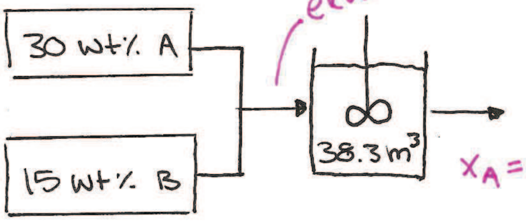
26

Ex.

$CH_2OHCH_2Cl + HCO_3 \rightarrow (CH_2OH)_2 + Cl^- + CO_2$ $\qquad A + B \rightarrow C + D + E$

$r = kC_AC_B$

ekvimolekylär feed



$m_c = 45 \ \frac{kg}{h}$

$X_A = 0.95$

$\rho = 10000 \ kg/m^3$

$M_A = 80 \ kg/kmol$

$M_B = 84$ "

$M_c = 62$ "

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

$$X_A F_{A_0} - kC_AC_BV = 0$$

$$\begin{cases} C_A = \frac{F_A}{q} = \frac{F_{A_0} - X_AF_{A_0}}{q} = C_{A_0}(1 - X_A) \\ C_B \equiv C_A \end{cases}$$

konc vid utflöde!

$$\rightarrow X_A F_{A_0} - k\left(\frac{F_{A_0}}{q}\right)^2 (1 - X_A)^2 V = 0$$

Vill veta k! Behöver F_{A_0}, q

$$F_c = \frac{m_c}{M_c} = 0.726 \ \frac{kmol}{h}$$

$$F_c = \cancel{F_{c_0}}^{0} + X_A F_{A_0} \rightarrow F_{A_0} = \frac{F_c}{X_A} = 0.764 \ \frac{kmol}{h}$$

$F_{B_0} \equiv F_{A_0}$ ty ekvimolekylär feed

$$q_A = \frac{0.764 \ kmol}{h} \bigg| \frac{80 \ kg \ A}{kmol} \bigg| \frac{100 \ kg \ sol.}{30 \ kg \ A} \bigg| \frac{m^3}{10^3 \ kg} = 0.204 \ \frac{m^3}{h}$$

$$q_B = \frac{0.764 \ kmol}{h} \bigg| \frac{84 \ kg \ B}{kmol} \bigg| \frac{100 \ kg \ sol.}{15 \ kg \ A} \bigg| \frac{m^3}{10^3 \ kg} = 0.428 \ \frac{m^3}{h}$$

$q = q_A + q_B$

$q = 0.632 \ m^3/h$

$$k = \frac{X_A F_{A_0}}{\left(\frac{F_{A_0}}{q}\right)^2 (1 - X_A)^2 V} = 5.19 \ \frac{m^3}{kmol \cdot h}$$

Vill även veta V: $\frac{dF_A}{dV} = r_j \rightarrow -F_{A_0}\frac{dX_A}{dV} = -kC_AC_B$

$$\rightarrow \ldots \Rightarrow V = 1.91 \ m^3$$