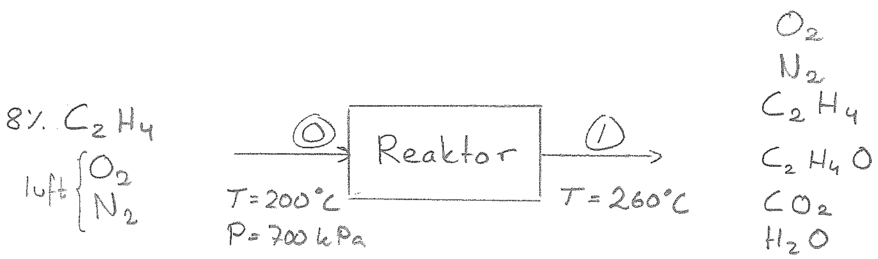
David Frisk

Material and Energy Balances

PP1



Reaktioner: 1. $C_2H_4 + \frac{1}{2} O_2 \longrightarrow C_2H_4O$

2. $C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$

$F^0_{tot} = 100 \text{ mol/s} \Rightarrow$

$F^0_{C_2H_4} = 8\% \cdot 100 = 8 \text{ mol/s}$

$F^0_{O_2} = 21\% \cdot (100\% - 8\%) \cdot 100 = 19,32 \text{ mol/s}$

$F^0_{N_2} = 79\% \cdot (100\% - 8\%) \cdot 100 = 72,68 \text{ mol/s}$

$R_1 = 40\% \cdot F^0_{C_2H_4} = 3,2 \text{ mol/s}$

$R_2 = 30\% \cdot F^0_{C_2H_4} = 2,4 \text{ mol/s}$

Kan nu beräkna sammansättningen i (1).

- $F^1_{C_2H_4} = F^0_{C_2H_4} + \nu_1 R_1 + \nu_2 R_2 = 8 - 3,2 - 2,4 = 2,4 \text{ mol/s}$
- $F^1_{O_2} = F^0_{O_2} + \nu_1 R_1 + \nu_2 R_2 = 19,32 - \frac{1}{2} \cdot 3,2 - 3 \cdot 2,4 = 10,52 \text{ mol/s}$
- $F^1_{N_2} = F^0_{N_2} = 72,68 \text{ mol/s}$
- $F^1_{C_2H_4O} = \nu_1 R_1 = 1 \cdot 3,2 = 3,2 \text{ mol/s}$
- $F^1_{CO_2} = \nu_2 R_2 = 2 \cdot 2,4 = 4,18 \text{ mol/s}$
- $F^1_{H_2O} = \nu_2 R_2 = 2 \cdot 2,4 = 4,8 \text{ mol/s}$

Vet nu sammansättningen av inflödet och utflödet:

In:
- C_2H_4 - 8 mol/s
- O_2 - 19,32 mol/s
- N_2 - 72,68 mol/s

Ut:
- C_2H_4 - 2,4 mol/s
- O_2 - 10,52 mol/s
- N_2 - 72,68 mol/s
- C_2H_4O - 3,2 mol/s
- CO_2 - 4,8 mol/s
- H_2O - 4,8 mol/s

David Frisk

För att bestämma hur mycket energi som frigörs, ställer vi upp en energibalans.

$\cancel{Ack}^{s.s} = In - Ut + Prod - Kylning$

$\Rightarrow \boxed{Kylning = In - Ut + Prod}$

$In = (T_{in} - T_{ref}) \cdot \sum_i F_i^0 \cdot \tilde{c}_{p_i} = (200-25)(8 \cdot 52{,}4 + 19{,}32 \cdot 30{,}1 + 72{,}68 \cdot 29{,}3)$
$= \underline{547{,}8 \text{ kW}}$

$Ut = (T_{ut} - T_{ref}) \cdot \sum_i F_i' \cdot \tilde{C}_{p_i} = (260-25)(2{,}4 \cdot 52{,}4 + 10{,}52 \cdot 30{,}1 + 72{,}68 \cdot 29{,}3 +$
$+ 3{,}2 \cdot 64{,}2 + 4{,}8 \cdot 41{,}6 + 4{,}8 \cdot 34{,}3) = \underline{738{,}3 \text{ kW}}$

Prod: $\Delta H_{R1} = \sum_i \nu_{1_i} \cdot (\Delta H_f^\circ)_i = (-1) \cdot 52{,}3 \cdot 10^3 + (-\frac{1}{2}) \cdot 0 + 1(-51{,}0 \cdot 10^3) =$
$= -103{,}3 \text{ kJ/mol}$

$\Delta H_{R_2} = \sum_i \nu_{2_i} \cdot (\Delta H_f^\circ)_i = (-1) \cdot 52{,}3 \cdot 10^3 + (-3) \cdot 0 + 2 \cdot (-393{,}7 \cdot 10^3) + 2(-241{,}8 \cdot 10^3) =$
$= -1323{,}3$

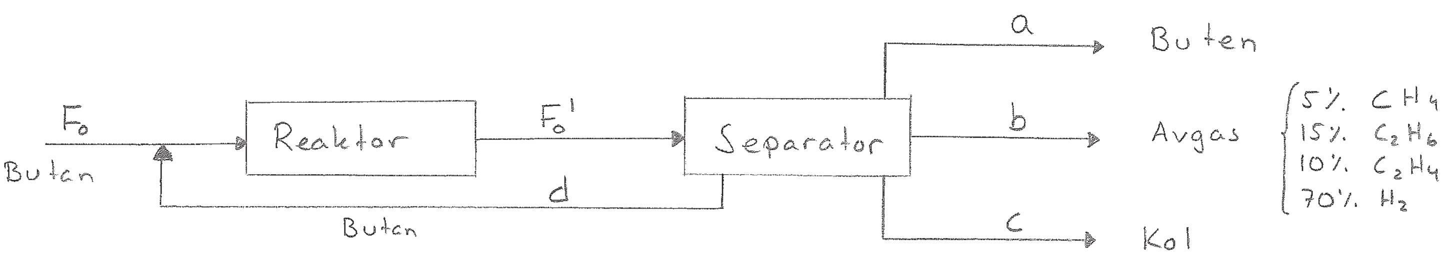
$\Rightarrow Prod = R_1 \cdot -\Delta H_{R1} + R_2 \cdot -\Delta H_{R2} = 3{,}2 \cdot 103{,}3 + 2{,}4 \cdot 1323{,}3 =$
$= \underline{3506{,}48 \text{ kW}}$

$\therefore Kylning = In - Ut + Prod = 547{,}8 - 738{,}3 + 3506{,}48 = 3315{,}98 \text{ kW}$

<u>Svar:</u> Reaktorn måste kylas med effekten <u>3316 kW</u> för att temperaturen ska hållas vid 260°C

David Frisk

PP2



Beräkna a, b, c, d, givet F_0.

5% av butan reagerar, utbytet av bildat buten är 50%

$\Rightarrow$ Reagerad butan: $0{,}05\,(F_0 + d)$
Bildad buten: $0{,}5 \cdot 0{,}05\,(F_0 + d)$

Materialbalanser över hela systemet $(0 = \text{In} - \text{Ut} + \text{Prod} - \text{kons})$

- Butan: $F_0 - 0 - 0{,}05\,(F_0 + d) = 0 \Rightarrow \underline{d = 19\,F_0 \text{ mol/s}}$
- Buten: $0 - a + 0{,}5 \cdot 0{,}05\,(F_0 + 19\,F_0) \Rightarrow \underline{a = 0{,}5\,F_0 \text{ mol/s}}$
- Väte: $10F_0 - 8 \cdot 0{,}5\,F_0 - b\,(4 \cdot 0{,}05 + 6 \cdot 0{,}15 + 4 \cdot 0{,}1 + 2 \cdot 0{,}7) = 0$

  $\Rightarrow \underline{b = 2{,}07\,F_0 \text{ mol/s}}$
- Kol: $4 \cdot F_0 - a \cdot 4 - b\,(0{,}05 + 2 \cdot 0{,}15 + 2 \cdot 0{,}1) - c = 0$

  $4F_0 - 2F_0 - 2{,}07\,F_0 \cdot 0{,}55 - c = 0$

  $\Rightarrow \underline{c = 0{,}86\,F_0 \text{ mol/s}}$

David Frisk

PP4

a) Materialbalans över hela systemet: $(In - Ut + Prod - Kons) = 0$

- Protein: $2{,}3 \cdot 0{,}45 - F^{ut}_{prot} + 0 - 0 = 0 \Rightarrow F^{ut}_{prot} = 1{,}035$ kg/min
- Fibrer: $2{,}3 \cdot 0{,}18 - F^{ut}_{fibr.} + 0 - 0 = 0 \Rightarrow F^{ut}_{fibr} = 0{,}414$ kg/min

$$\begin{cases} F^{ut}_{tot} = 1{,}035 + 0{,}414 + F^{ut}_{hexan} \\ F^{ut}_{hexan} = 0{,}03 \cdot F^{ut}_{tot} \end{cases} \Rightarrow F^{ut}_{tot} = \frac{1{,}035 + 0{,}414}{1 - 0{,}03} = 1{,}494 \text{ kg/min}$$

Andel Protein: $\frac{1{,}035}{1{,}494} = 69{,}3\%$

Andel Fibrer: $\frac{0{,}414}{1{,}494} = 27{,}7\%$

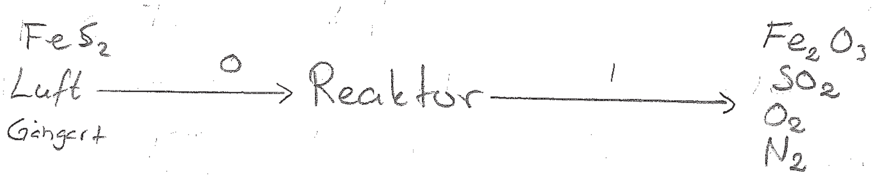
Andel hexan: 3%

b) Olja: $2{,}3 \cdot 0{,}37 - F^{ut}_{olja} = 0 \Rightarrow F^{ut}_{olja} = 0{,}851$ kg/min

c) Hexan: $F^{5}_{hex} - 0{,}03 \cdot 1{,}494 = 0 \Rightarrow F^{5}_{hex} = 0{,}045$ kg/min

Svar: a) $F^2 = 1{,}494$ kg/min b) $F^6 = 0{,}851$ kg/min, $F^5 = 0{,}045$ kg/min

PP5



R: $4FeS_2 + 11O_2 \rightarrow 2Fe_2O_3 + 8SO_2$

Materialbalans:

FeS_2: $F^0_{FeS_2} - 4R = 0 \Rightarrow R = \frac{1}{4} F^0_{FeS_2} = \frac{1}{4} \cdot 0{,}85 \cdot \frac{1000}{120} \cdot 10^3 = 1770{,}8$ mol/h

$F^0_{O_2} = \frac{11}{4} \cdot F^0_{FeS_2} \cdot 3 = 58{,}4$ kmol/h

$\Rightarrow F^0_{N_2} = \frac{79}{21} \cdot F^0_{O_2} = 219{,}8$ kmol/h

$\Rightarrow F'_{O_2} = \frac{2}{3} \cdot F^0_{O_2} = 38{,}9$ kmol/h

$F'_{N_2} = F^0_{N_2} = 219{,}8$ kmol/h

$F'_{SO_2} = 8R = 14{,}2$ kmol/h

Fast form $\left(F'_{Fe_2O_3} = 2R = 3{,}542 \text{ kmol/h}\right)$

$F'_{tot} = 273$ kmol/h		
Andel SO_2:	$\frac{14{,}2}{273}$	5,2%
Andel O_2:	$\frac{38{,}9}{273}$	14,3%
Andel N_2:	$\frac{219{,}8}{273}$	80,5%

$F^0_{FeS_2} = 0{,}85 \cdot \frac{1000}{120} \cdot 10^3 = 7083$ mol/h

$F^0_{Gångert} = 0{,}15 \cdot \frac{1000}{120} \cdot 10^3 = 1250$ mol/h

F'

PP5 forts. Energibalans: In − Ut + Prod = 0

▸ Prod: $R \cdot (-\Delta H_R) = 1770{,}8 \cdot 1659 \cdot 10^3 \frac{J}{h} = 2{,}938 \cdot 10^9 \, J/h$ = kW

▸ In: $In = (800 - 800) \, F_j^{\circ} \tilde{C}_{p_j} = 0$

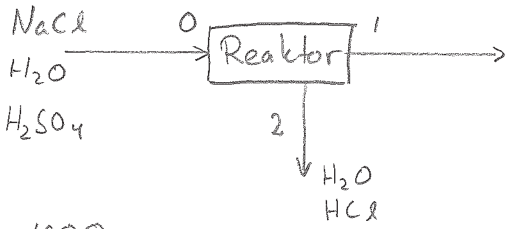
▸ Ut: $Ut = (T_{ut} - 800) \cdot \sum F_j^1 \cdot \tilde{C}_{p_j} = (T_{ut} - 800) \cdot$ $\left[\frac{mol}{h} \cdot K \cdot \frac{J}{mol \cdot K} = J/h\right]$

$= (T_{ut} - 800) \cdot (38{,}9 \cdot 35 + 219{,}8 \cdot 35 + 14{,}2 \cdot 40 + 3{,}542 \cdot 180 + 150 \cdot 20) \cdot 10^3$

$= (T_{ut} - 800) = 10{,}56 \cdot 10^6 \, J/h$

$\Rightarrow T_{ut} = 800 + \frac{2{,}938 \cdot 10^9}{11{,}51 \cdot 10^6} \, K = 1078 \, K$

PP10



	Massprocent	Molprocent
Na_2SO_4	91,48 %	80,08 %
$NaHSO_4$	4,78 %	4,95 %
$NaCl$	1,98 %	4,21 %
H_2O	1,36 %	9,39 %
HCl	0,40 %	1,36 %

R_1: $NaCl + H_2SO_4 \rightarrow NaHSO_4 + HCl$

R_2: $NaCl + NaHSO_4 \rightarrow Na_2SO_4 + HCl$

$N^{\circ}_{NaCl} = \frac{1000}{58{,}44} = 17{,}11 \, kmol$

(1) NaCl: $N^{\circ}_{NaCl} - N^1_{NaCl} - R_1 - R_2 = 0 \Rightarrow 17{,}11 - R_1 - R_2 = 0{,}0421 \cdot N^1$

(2) H_2SO_4: $N^{\circ}_{H_2SO_4} - N^1_{H_2SO_4} - R_1 = 0 \Rightarrow N^{\circ}_{H_2SO_4} = R_1$

(3) $NaHSO_4$: $N^{\circ}_{NaHSO_4} - N^1_{NaHSO_4} + R_1 - R_2 = 0 \Rightarrow R_1 - R_2 = 0{,}0495 \, N^1$

(4) H_2O: $N^{\circ}_{H_2O} - N^1_{H_2O} - N^2_{H_2O} = 0 \Rightarrow N^{\circ}_{H_2O} = N^2_{H_2O} + 0{,}0939 \cdot N^1$

(5) HCl: $N^{\circ}_{HCl} - N^1_{HCl} - N^2_{HCl} + R_1 + R_2 = 0 \Rightarrow R_1 + R_2 = N^2_{HCl} + 0{,}0136 \cdot N^1$

(6) Na_2SO_4: $N^{\circ}_{Na_2SO_4} - N^1_{Na_2SO_4} + R_2 = 0 \Rightarrow R_2 = 0{,}8088 \cdot N^1$

(1),(3),(6) ⇒ $\begin{cases} R_1 + R_2 + 0{,}0421 \, N^1 = 17{,}11 \\ R_1 - R_2 - 0{,}0495 \, N^1 = 0 \\ 0 + R_2 - 0{,}8008 \, N^1 = 0 \end{cases}$ AirWolf ⇒ $R_1 = 8{,}592$ kmol, $R_2 = 8{,}092$ kmol, $N^1 = 10{,}105$ kmol

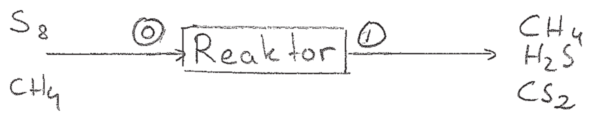
Tillsatt H_2SO_4: $N^{\circ}_{H_2SO_4} = R_1 = 8{,}592 \, kmol \Rightarrow m = 842{,}76 \, kg$ ⇒ Tillsatt syra = $\frac{842{,}76}{0{,}75} = 1124 \, kg$

Bildad HCl: $R^1 + R^2 - 0{,}0136 \cdot N^1 = 16{,}55 \, kmol$

Andel salt i R_1: $\frac{R_1}{N^{\circ}_{NaCl}} = \frac{8{,}592}{17{,}11} = 50{,}21 \%$

David Frisk

PP11 a)



R: $CH_4 + \frac{1}{2} S_8 \rightarrow CS_2 + 2H_2S$

CS_2 $\quad 0 - N^1_{CS_2} + R = 0 \Rightarrow R = 1\,mol$

H_2S $\quad 0 - N^1_{H_2S} + 2R = 0 \Rightarrow N^1_{H_2S} = 2mol$

S_8 $\quad N^0_{S_8} - \frac{1}{2} R = 0 \Rightarrow N^0_{S_8} = \frac{1}{2}\,mol$

CH_4 $\quad N^0_{CH_4} = 3 \cdot N^0_{S_8} = \frac{3}{2}\,mol \qquad N^0_{CH_4} - N^1_{CH_4} - R = 0 \Rightarrow N^1_{CH_4} = \frac{1}{2}\,mol$

Energibalans: In − Ut + Prod + Värmning = 0

$In = \left(N^0_{S_8} \cdot C_{P_{S_8(l)}}\right)(220-175) = 659,25$

$Ut = \left(N^1_{CH_4} \cdot C_{P_{CH_4}} + N^1_{H_2S} \cdot C_{P_{H_2S}} + N^1_{CS_2} \cdot C_{P_{CS_2}}\right)(250-175) = 9907,5\,J$

Prod = −92000

Värmning = Ut − In − Prod = 9907,5 − 659,25 + 92000 = 101,25 kJ

b) $E_{metan} = (700-175) \cdot N^0_{CH_4} \cdot C_{P_{CH_4}} = 32917,5\,J$

$E_{svavel} = (700-250) \cdot N^0_{S_8} \cdot C_{P_{S_8(g)}} + N^0_{S_8} \cdot \Delta H_{vap_{S_8}} + (250-220)\, N^0_{S_8} \cdot C_{P_{S_8(l)}} = 12154,5\,J$

Till värmeväxlare A: $\frac{12154,5}{12154,5 + 32917,5} = 0,27 = 27\,\%$

Svar: a) 101,25 kJ, b) 27% till A.

Alt: Energibalans: $0 = Q + \int_{700}^{250} \sum_{in} N_i \cdot C_{p_i}\, dT + R \cdot (-\Delta H_{rxn}) - \int_{250}^{T_{in}} \sum_{ut} N_u \cdot C_{p_u}\, dT$

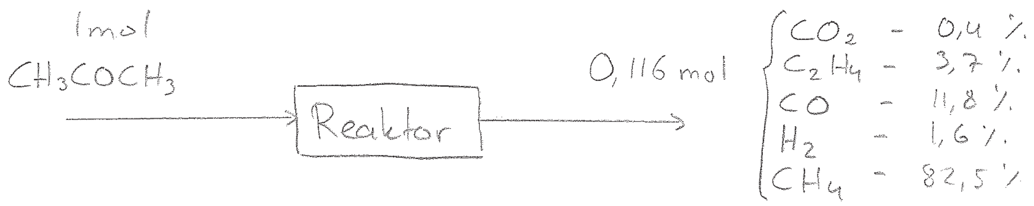
$Q_A = \Delta T \sum_i C_{p_i} n_i = (T_{in} - 250)(0,27 \cdot \frac{1}{2} \cdot 41,8 + 0,27 \cdot 2 \cdot 39,7 + 0,27 \cdot 1 \cdot 31,8) = 12155\,J$

$\Rightarrow T_{in} = 590,7\,°C$

Q = Ut − In − Rxn = 45046 − 35730 + 92000 = 101316 J/mol CS_2

David Frisk

PP12



- R_1: $CH_3COCH_3 \rightarrow CH_4 + CH_2{=}CO$
- R_2: $2\,CH_2{-}CO \rightarrow C_2H_4 + 2CO$
- R_3: $CH_3COCH_3 \rightarrow 3H_2 + CO + 2C$

CH_4: $0 - 0{,}116 \cdot 0{,}825 + R_1 = 0 \Rightarrow R_1 = 0{,}0957$ mol

H_2: $0 - 0{,}116 \cdot 0{,}016 + 3R_3 = 0 \Rightarrow R_3 = 0{,}000619$ mol

C_2H_4: $0 - 0{,}116 \cdot 0{,}037 + R_2 = 0 \Rightarrow R_2 = 0{,}004292$ mol

Reagerad Aceton: $R_1 + R_3 = 0{,}0963$ mol $= 9{,}63\%$ av inflödet.

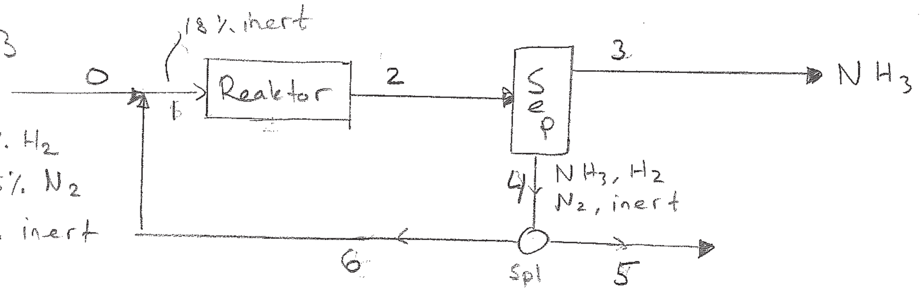
Bildad keten: $R_1 - 2R_2 = 0{,}0871$ mol

Andel reagerad aceton som ger ketener: $\frac{0{,}0871}{0{,}0963} = 90{,}45\%$.

David Frisk

PP13

74% H_2
24,5% N_2
1,5% inert



1. $F^3_{NH_3} = 0{,}75 \cdot F^2_{NH_3}$

(2. $F^4_{NH_3} = 0{,}25 \cdot F^2_{NH_3}$)

3. $F^2_{N_2} = 0{,}35 \cdot F^1_{N_2}$

Frihetsgrader =

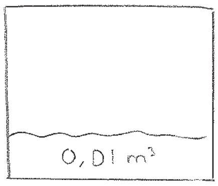
= #Variabler − # Balanser − # Sammansättn. − Hjälpsamband − Räknebas

	Reaktor	Separator	Splitter	Process	Tot
# Variabler	4+4+1=9	4+4+1=9	4+4+4=12	24+1=25	9
# Balanser	−4	−4	−4	−12	−4
Sammansättn.	−1	0	0	−3	−2
Hjälpsamband					
1.	0	−1	0	−1	
3	−1	0	0	−1	
Räknebas	−1	−1	−1	−1	−1
	2	3	7	7	2

David Frisk

Ideala reaktorer - molbalanser

(IRM) 4



$A + B \rightarrow R \quad , \quad r = k \cdot c_A c_B$

$c_{A,0} = 0,5 \text{ kmol/m}^3$
$c_{B,0} = 0,01 \text{ kmol/m}^3$
$k = 5,56 \cdot 10^{-3} \text{ m}^3/\text{kmol s}^{-1}$

$r_0 = k \cdot c_{A,0} \cdot c_{B,0} =$

$= 0,5 \cdot 0,01 \cdot 5,56 \cdot 10^{-3} \left\{ \frac{\text{kmol}}{\text{m}^3} \cdot \frac{\text{kmol}}{\text{m}^3} \cdot \frac{\text{m}^3}{\text{kmol} \cdot \text{s}} \right\} = 2,78 \cdot 10^{-5} \text{ kmol/m}^3 \cdot \text{s}$

Vid $t = 0$ tillförs $-\left(\frac{\partial N}{\partial t}\right) = (r_0 \cdot V) = -2,78 \cdot 10^{-5} \cdot 0,01 = \underline{2,78 \cdot 10^{-4} \text{ mol/s}}$ ämne B

Satsreaktorekvationen: $\nu_j \cdot r = \frac{\partial c_i}{\partial t} \Rightarrow \frac{\partial c_A}{\partial t} = -1 \cdot r = -k \cdot c_A \cdot c_B$

$\Rightarrow \int_{c_{A,0}}^{c_A} \frac{\partial c_A}{c_A} = -k \int_0^t c_B \, dt \Rightarrow \ln \frac{c_A}{c_{A,0}} = -k \, c_B \, t$ Lös ut $c_A = c_A(t)$

$c_A = c_{A,0} \, e^{-k c_B t}$. $t = 2\text{h} = 7200 \text{ s} \Rightarrow c_A = 0,5 \cdot e^{-k \cdot 0,01 \cdot 7200} = 0,335 \text{ kmol/m}^3$

$r_{2h} = k \cdot c_{A,2h} \cdot c_B = 1,86 \cdot 10^{-5} \text{ kmol/m}^3 \cdot \text{s}$

Vid $t = 2\text{h}$ (7200 s) tillförs $\frac{\partial N_B}{\partial t} = r_{2h} \cdot V = \underline{1,86^{-4} \text{ mol/s}}$ ämne B

(IRM) 5:

$A \rightarrow B \, . \quad r = \frac{k \, c_A}{1 + K_A \cdot c_A} \quad , \quad k = 1,5 \text{ s}^{-1}, \; K_A = 10 \text{ m}^3/\text{kmol}$

$c_{A0} = 20 \text{ kmol/m}^3, \quad c_{B0} = 0$

$\frac{\partial c_A}{\partial t} = -\frac{k \cdot c_A}{1 + K_A \cdot c_A}$ Separera och integrera.

$\Rightarrow \int_{c_{A0}}^{c_A} \frac{1 + K_A \cdot c_A}{c_A} \, dc_A = -k \int_0^t dt$

$\int_{c_{A0}}^{c_A} \frac{1}{c_A} \, dc_A + \int_{c_{A0}}^{c_A} K_A = -k \int_0^t dt \Rightarrow \ln \frac{c_A}{c_{A0}} + K(c_A - c_{A0}) = -k \, t$

$c_A = \frac{1}{2} c_{A0} \Rightarrow \frac{\ln\left(\frac{\frac{1}{2} c_{A0}}{c_{A0}}\right) + K_A\left(\frac{1}{2} c_{A0} - c_{A0}\right)}{-k} = t$

$\Rightarrow t = -\frac{\ln \frac{1}{2} - K_A \cdot \frac{1}{2} \cdot 20}{1,5} = 67,1 \text{ s}$

David Frisk

(IRM) 6 $A \rightarrow B$, $r = k \cdot c_A$, där $k = 1\,s^{-1}$

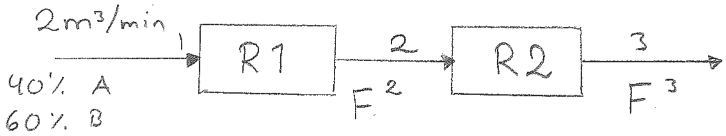
$$\frac{\partial c_A}{\partial t} = -r = -k\,c_A \qquad \text{Sep, Int} \Rightarrow \int_{c_{A,0}}^{c_A} \frac{dc_A}{c_A} = -\int_0^t dt$$

$$\Rightarrow \ln \frac{c_A}{c_{A0}} = -t \quad \Rightarrow \quad c_A = c_{A0}\, e^{-t}$$

$$X_1 = \frac{\text{mol reagerat}}{\text{mol matat}} = 0{,}8 \quad ; \quad 0{,}2\, c_{A0} = c_{A0}\, e^{-t} \Rightarrow$$

$$\Rightarrow \ln 0{,}2 = -t \quad \Rightarrow \quad t = -\ln 0{,}2 = 1{,}609\,s$$

(IRM) 7 $A + 2B \rightarrow C$



$$\dot{n} = \frac{p\dot{V}}{RT} = \frac{1013 \cdot 10^3 \cdot 2}{R \cdot (227 + 273{,}15)} = 487{,}2\ \text{mol/min}$$

$F_A^1 = 195$ mol/min $\qquad X_A^2 = 0{,}40 = \dfrac{\text{mol A reg}}{\text{mol A in}} \Rightarrow$ mol A kvar, 2 $= 0{,}6 \cdot F_A^1 = 117$ mol/min

$F_B^1 = 292$ mol/min $\qquad \Rightarrow R_1 = 78$ mol/min $\Rightarrow F_B^2 = 136$ mol/min

$X_A^3 = 0{,}60 \Rightarrow$ mol A kvar, 3 $= 0{,}4 \cdot F_A^1 = 78$ mol/min

$R_{tot} = 117$ mol/min $\Rightarrow F_B^3 = F_B^1 - 2R_{tot} = 58$ mol/min

$\therefore$

$F_A^1 = 195$ mol/min	$F_A^2 = 117$ mol/min	$F_A^3 = 78$ mol/min
$F_B^1 = 292$ mol/min	$F_B^2 = 136$ mol/min	$F_B^3 = 58$ mol/min

Reaktor 1

$X_A = 0{,}4 \Rightarrow r = 20$ mol/m³·s $\quad ; \quad F_A^1 = \frac{195}{60} = 3{,}248$ mol/s

Materialbalans: $0 = F_A^1 - F_A^2 + \nu_A \cdot r_1 \cdot V_{r,1} = F_A^1 - F_A^1(1 - X_{1,A}) = r_1 \cdot V_{r_1}$

$$\Rightarrow V_{r_1} = \frac{X_{1,A} \cdot F_A^1}{r_1} = 0{,}065\ m^3$$

Reaktor 2

Materialbalans: $F_A^2 - F_A^1 \cdot (1 - 0{,}6) = r_2 \cdot V_{r,2} \qquad r_2\big|_{X=0{,}6} = 10$ mol/m³·s

$$V_{r,2} = \frac{F_A^1(1-0{,}4) - F_A^1(1-0{,}6)}{r_2} = \frac{F_A^1(1 - 0{,}4 - 1 + 0{,}6)}{r_2} =$$

$$= \frac{3{,}248 \cdot 0{,}2}{10} = 0{,}065\,m^3$$

Svar: $V_{r_1} = V_{r_2} = 0{,}065\,m^3$

David Frisk

(IRM) 8 $\quad 2A \rightarrow R \quad , r = k c_A^2$

$c_{A0} = 2{,}20$ kmol/m³ $\quad$ Inflöde: $0{,}8 \cdot 10^{-3}$ m³/s $\quad X_A = 0{,}7$

Parrallellt flöde: $\quad q_f = 0{,}4 \cdot 10^{-3}$ m³/s och $V_r = 1{,}6$ m³

MB: $\quad F_A^0 - F_A^1 - 2R = 0 \quad , R = rV_r = k c_A^2 V_r$

$$\Rightarrow q_f c_{A0} - q_f c_A - 2k c_A^2 V_r = 0 \quad , \quad c_A = c_{A0}(1-x_A)$$

$$\Rightarrow q_f c_{A0} - q_f c_{A0}(1-x_A) - 2k c_{A0}^2 (1-x_A)^2 V_r = 0$$

$$\Rightarrow k = \frac{q_f(1-(1-X_A))}{2 V_r c_{A0}(1-X_A)^2} = \underline{4{,}42 \cdot 10^{-7}} \text{ m}^3/\text{mol}\cdot\text{s}$$

a) Tank 1 $\quad c_{A0} = 2{,}2$ kmol/m³ , $V_r = 1{,}6$ m³ , $q_f = 0{,}8 \cdot 10^{-3}$ m³/s

MB: $\quad F_A^0 - F_A^1 - 2R = 0$

$$q_f c_{A0} - q_f c_{A0}(1-x_A^1) - 2k c_{A0}^2 (1-x_A^1)^2 V_r = 0 \qquad \Rightarrow \underline{x_A^1 = 0{,}6054}$$

Tank 2 $\quad c_A^1 = 2{,}2 \cdot (1-x_A^1)$ kmol/m³, $V_r = 1{,}6$ m³ , $q_f = 0{,}8 \cdot 10^{-3}$ m³/s

MB: $\quad F_A^1 - F_A^2 - 2R = 0$

$$q_f \cdot c_A^1 - q_f \cdot c_A^2 - 2k (c_A^2)^2 \cdot V_r = 0 \quad , \quad c_A^1 = c_{A0}(1-x_A^1) \quad c_A^2 = c_{A0}(1-X_A^2)$$

$$\Rightarrow q_f c_{A0}(1-x_A^1) - q_f c_{A0}(1-x_A^2) - 2kV_r (c_{A0}(1-x_A^2))^2 = 0$$

$$\Rightarrow q_f (1-x_A^1 - 1 + x_A^2) = 2kV_r c_{A0} (1-x_A^2)^2 \qquad \Rightarrow \underline{x_A^2 = 0{,}7851}$$

b) Satsreaktor $\quad V = 2 \cdot 1{,}6 = 3{,}2$ m³ , $q_f = 0{,}8 \cdot 10^{-3}$ m³/s , $c_{A0} = 2200$ mol/m³

$$t_{cykel} = t_{reak} + 15 \cdot 60 \quad , \quad t_{cykel} = \frac{V_r}{q_{tot}/2} = \frac{1{,}6}{0{,}8 \cdot 10^{-3}/2} = 4000 \text{ s}$$

$$\Rightarrow t_{reak} = 4000 - 15 \cdot 60 = 3100 \text{ s}$$

$$\frac{dc_A}{dt} = \nu \cdot r = \nu \cdot k c_A^2 \quad , \text{ sep. int} \Rightarrow \int \frac{1}{c_A^2} dc_A = -2k \int dt$$

Integrera från $0 \rightarrow t$, $0 \rightarrow c_A$

$$\int_{c_{A0}}^{c_A} \frac{1}{c_A^2} dc_A = -2kt \Rightarrow \left[\frac{1}{c}\right]_{c_{A0}}^{c_A} = 2kt \Rightarrow \frac{1}{c_A} - \frac{1}{c_{A0}} = 2kt$$

$$\Rightarrow \frac{1}{c_A} = 2kt + \frac{1}{c_{A0}} \Rightarrow c_A = \frac{1}{2kt + \frac{1}{c_{A0}}} = \left(2 \cdot k \cdot 3100 + \frac{1}{2200}\right)^{-1} = 313 \text{ mol/m}^3$$

$$x_A = \frac{(c_{A0} - c_A)}{c_{A0}} = 1 - \frac{c_A}{c_{A0}} = 1 - \frac{313}{2200} = 0{,}8577$$

Svar $\quad$ a) $X_A = 0{,}7851 \quad$ b) $X_A = 0{,}8577$

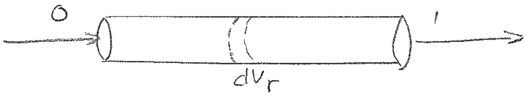
David Frisk

(RD)4 $4PH_{3(g)} \rightarrow P_4(g) + 6H_2(g)$

Hur stor tubreaktor krävs för att vid 4,6 bar, 650°C få $X = 0{,}80$ vid $q_f = 2\,mol/h$

$r = k\,C_{PH_3}$, $k = 10^{-3}/s$ (650°C)

$PH_3 \rightarrow \frac{1}{4} P_4 + \frac{6}{4} H_2$



$$C_A = \frac{N_A(X)}{N_{tot}(X)} \frac{P}{RT}$$

$$F_A^\circ(1-x_A) - F_A^\circ(1-x_A-dx_A) + \nu_A \cdot r \cdot dV_r = 0$$

$$\Rightarrow F_A^\circ \cdot dx_A = 4k \cdot c_A \cdot dV_r \qquad (1)$$

$$c_A = \frac{P_A}{RT} = \frac{F_A}{F_{tot}} \cdot \frac{P_{tot}}{RT}$$ Behöver bestämma F_{tot}

$$\left.\begin{aligned} F_A &= F_A^\circ(1-x_A) \\ F_B &= \frac{1}{4} \cdot F_A^\circ \cdot x_A \\ F_C &= \frac{6}{4} F_A^\circ \cdot x_A \end{aligned}\right\} \quad F_{tot} = F_A^\circ - F_A^\circ x_A + \frac{1}{4} F_A^\circ x_A + \frac{6}{4} F_A^\circ x_A = F_A^\circ + F_A^\circ x_A \cdot \frac{3}{4}$$

$$\Rightarrow C_A = \frac{F_A^\circ(1-x_A)}{F_A^\circ(1+\frac{3}{4}x_A)} \cdot \frac{P_{tot}}{RT}$$ Sätts in i (1):

$$F_A^\circ dx_A = 4k \frac{(1-x_A)}{1+\frac{3}{4}x_A} \cdot \frac{P_{tot}}{RT} dV_r$$ Separera och integrera:

$$\int_0^{0,8} \frac{dx_A}{\frac{1-x_A}{1+\frac{3}{4}x_A}} = \frac{4k P_{tot}}{F_A^\circ RT} \int_0^V dV_r \Rightarrow V_r = \frac{F_A^\circ RT}{4k P_{tot}} \int_0^{0,8} \frac{1+\frac{3}{4}x_A}{1-x_A} dx_A =$$

$$= \frac{F_A^\circ RT}{4k P_{tot}} \int_0^{0,8} \frac{1}{1-x_A} + \frac{\frac{3}{4}x_A}{1-x_A} dx_A \overset{(*)}{=} \frac{F_A^\circ RT}{4k P_{tot}} \cdot 2{,}2165 = 5{,}137 \cdot 10^{-3}\ m^3$$

<u>Svar: $V_r = 5{,}14\ dm^3$</u>

$$(*) = \int_0^{0,8} \frac{1}{1-x} + \frac{\frac{3}{4}x}{1-x} dx \overset{BETA}{=} \left[-\ln(1-x) + \frac{3}{4} \cdot \left(\frac{x}{-1} - \frac{1}{(-1)^2}\ln(1-x)\right)\right]_0^{0,8} =$$

$$= \left[-\frac{3}{4}x - \left(\ln(1-x) - \frac{3}{4}\ln(1-x)\right)\right]_0^{0,8} = \left[-\frac{3}{4}x - 1{,}75\ln(1-x)\right]_0^{0,8} =$$

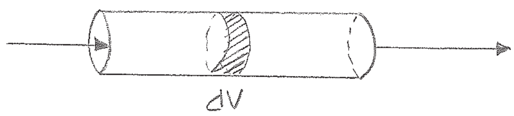
$$= \left(-\frac{3}{4} \cdot 0{,}8 - 1{,}75\ln(1-0{,}8)\right) - (0-0) = 2{,}2165$$

David Frisk

(RD)8 $SO_2 + \frac{1}{2} O_2 \rightleftharpoons SO_3$ $T = 460°C$ $\dot{m} = 2\ kg/s$

Inflöde: 8 vol% SO_2, 12 vol% O_2 och 80 vol% N_2

$X_{SO_2} = 0,6$



Materialbalans över kontrollvolymen dV:

$$F^\circ_{SO_2}(1 - X_{SO_2}) - F^\circ_{SO_2}(1 - (X_{SO_2} + dX_{SO_2})) - r\,dV_r = 0$$

$$F^\circ_{SO_2}(\cancel{1 - X_{SO_2}} \cancel{- 1 + X_{SO_2}} + dX_{SO_2}) - r\,dV_r = 0$$

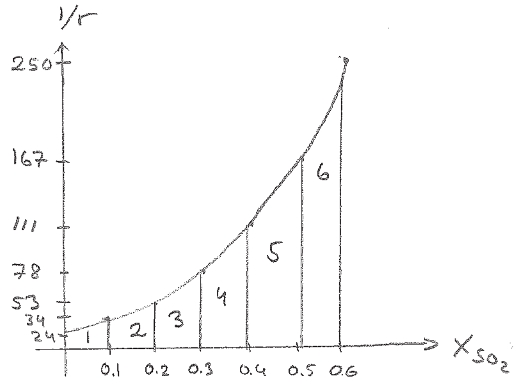
$$F^\circ_{SO_2}\, dX_{SO_2} - r\,dV_r = 0 \quad \Rightarrow \quad V_r = F^\circ_{SO_2} \cdot \int_0^{0,6} \frac{dX_{SO_2}}{r} \quad ? \qquad (1)$$

V_r är vikten av katalysatorn. ?

$F^\circ_{SO_2} = ?$ $$Y^{vikt}_{SO_2} = \frac{0,08 \cdot 64}{0,08 \cdot 64 + 0,12 \cdot 32 + 0,8 \cdot 28} = 0,1633$$

$$F^\circ_{SO_2} = 0,1633 \cdot 2\ kg/s = 0,3265\ kg/s = \frac{0,3265}{64 \cdot 10^{-3}} = 5,1020\ mol/s$$

$$\int_0^{0,6} \frac{1}{r}\, dX_{SO_2} = \sum_{i=1}^{6} A_i$$



$A_1 = 0,1 \cdot 24 + 0,1 \cdot (34 - 24)/2 = 2,9\ kg\,s/mol$

$A_2 = 0,1(34 + \frac{1}{2}(53 - 34)) = 4,35\ kg\,s/mol$

$A_3 = 0,1(53 + \frac{1}{2}(78 - 53)) = 6,55\ kg\,s/mol$

$A_4 = 0,1(78 + \frac{1}{2}(111 - 78)) = 9,45\ kg\,s/mol$

$A_5 = 0,1(111 + \frac{1}{2}(167 - 111)) = 13,9\ kg\,s/mol$

$A_5 = 0,1(167 + \frac{1}{2}(250 - 167)) = 20,85\ kg\,s/mol$

$$\Rightarrow \int_0^{0,6} \frac{1}{r}\, dX_{SO_2} = 2,9 + \ldots + 20,85 = 58\ kg\,s/mol$$

(1) ger: $$V_r = F^\circ_{SO_2} \cdot \int_0^{0,6} \frac{1}{r}\, dX_{SO_2} = 5,1020 \cdot 58 = \left\{\frac{kg \cdot s}{mol} \cdot \frac{mol}{s}\right\} = \underline{296\ kg}$$

David Frisk

(RD) 9 Tubreaktor, 3,3 cm diameter, 80 cm lång.

$A \rightarrow \underset{B}{CH_4} + \underset{C}{CO}$

$F_{A0} = 3,16 \cdot 10^{-4}$ mol/s $\Rightarrow X_A = 0,13$

$F_{A0} = 1,33 \cdot 10^{-4}$ mol/s $\Rightarrow X_A = 0,24$

$F_{A0} = 0,682 \cdot 10^{-4}$ mol/s $\Rightarrow X_A = 0,35$

$r = r(c_A)$

$r = k \cdot c_A$ eller $r = k \cdot c_A^2$

$V = \pi r^2 \cdot l = \pi \cdot \left(\frac{0,033}{2}\right)^2 \cdot 0,8 = 0,00068 \text{ m}^3$

$r = k c_A^2$ – Testa andra ordningen

$$F_A^{\circ}(1-X_A) - F_A^{\circ}(1-X_A-dX_A) - r\,dV_r = 0 \quad , \quad r = k c_A^2$$

$$F_A^{\circ} dX_A = k c_A^2 dV_r$$

$$C_A = \frac{P_A}{RT} = \frac{F_A}{F_{tot}} \cdot \frac{P_{tot}}{RT}$$

$$\left.\begin{aligned} F_A &= F_{A0}(1-X_A) \\ F_B &= F_A^{\circ} \cdot X_A \\ F_C &= F_A^{\circ} \cdot X_A \end{aligned}\right\} \quad F_{tot} = F_{A0}(1 - X_A + X_A + X_A) = F_{A0}(1+X_A)$$

$$\Rightarrow C_A = \frac{F_{A0}(1-X_A)}{F_{A0}(1+X_A)} \frac{P}{RT} = \frac{(1-X_A)}{(1+X_A)} \frac{P}{RT}$$

$$\Rightarrow F_{A0}\, dX_A = k \left(\frac{1-X_A}{1+X_A} \frac{P}{RT}\right)^2 dV_r \qquad \text{Sep Int}$$

$$\int_0^{X_A} \frac{(1+X_A)^2}{(1-X_A)^2} dX_A = \frac{kP^2}{F_{A0} R^2 T^2} \int_0^V dV_r \Rightarrow k = F_{A0} \underbrace{\frac{R^2T^2}{P^2V}}_{C_1} \int_0^{X_A} \frac{(1+X_A)^2}{(1-X_A)^2} dX_A$$

Försök 1: $k = C_1 \cdot 3,16 \cdot 10^{-4} \cdot \int_0^{0,13} \frac{(1+X_A)^2}{(1-X_A)^2} dX_A = 5,39 \cdot 10^{-5} C_1$

Försök 2: $k\big|_{X_A = 0,24,\ F_{A0} = 1,33 \cdot 10^{-4} \text{mol/s}} = 5,39 \cdot 10^{-5} C_1$ Samma ⇒ Rätt!

Försök 3: $k\big|_{X_A = 0,35,\ F_{A0} = 0,682 \cdot 10^{-4} \text{mol/s}} = 5,32 \cdot 10^{-5} C_1$ Samma!!!

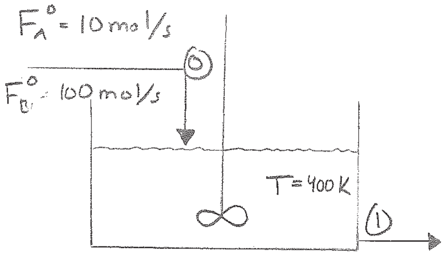
$$C_1 = \frac{R^2T^2}{P^2V} = 6,157 \Rightarrow k = 6,157 \cdot 5,39 \cdot 10^{-5} = 3,32 \cdot 10^{-4}$$

Enhet: $k = r \cdot \frac{1}{C_A^2} : \frac{\text{mol}}{\text{m}^3 \cdot \text{s}} \cdot \left(\frac{\text{m}^3}{\text{mol}}\right)^2 = \frac{\text{mol}\ \text{m}^6}{\text{m}^3\text{s}\ \text{mol}^2} = \text{m}^3/\text{s} \cdot \text{mol}$

Svar: $k = 3,32 \cdot 10^{-4}$ m³/s·mol

David Frisk

(IRV) 3



$A + 3B \rightarrow 2C \quad , \; r = k c_A c_B$

$F_A^1 = F_A^0(1-x) = \underline{5 \text{ mol/s}}$

a) Materialbalans över reaktorn:

A: $F_A^0 - F_A^1 - R = 0 \quad \Rightarrow \quad R = 5 \text{ mol/s}$

B: $F_B^0 - F_B^1 - 3R = 0 \quad \Rightarrow F_B^1 = F_B^0 - 3R = 100 - 15 = \underline{85 \text{ mol/s}}$

C: $\cancel{F_C^0} - F_C^1 + 2R = 0 \quad \Rightarrow F_C^1 = 2R = \underline{10 \text{ mol/s}}$

b) Beräkna k vid 400 K $\qquad R = rV = k c_A c_B V \qquad (1)$

Koncentrationerna beräknas vid utflödet.

$$c_A = \frac{F_A^1}{\sum F^1} \cdot \frac{P}{RT} = \frac{5}{100} \cdot \frac{101325}{8{,}3145 \cdot 400} = 1{,}5233 \text{ mol/m}^3$$

$$c_B = \frac{F_B^1}{\sum F^1} \cdot \frac{P}{RT} = \frac{85}{100} \cdot \frac{101325}{8{,}3145 \cdot 400} = 25{,}8965 \text{ mol/m}^3$$

$$(1) \Rightarrow \quad k = \frac{R}{c_A c_B \cdot V} = 0{,}127 \left\{ \frac{\cancel{mol}}{s} \cdot \frac{\cancel{m^3}}{mol} \cdot \frac{m^3}{\cancel{mol}} \cdot \frac{1}{\cancel{m^3}} \right\} = 0{,}127 \text{ m}^3/\text{s} \cdot \text{mol}$$

c) Bestäm inflödestemperaturen. $\qquad$ Värmebalans

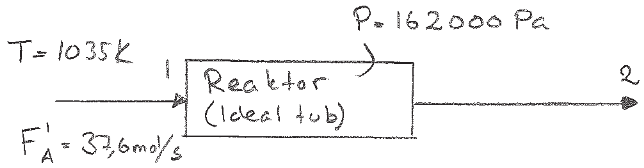
$$0 = \sum_{in} N_i \cdot \int_{T_{ref}}^{T_{in}} C_{p,i} \, dT - \sum_{ut} N_i \cdot \int_{T_{ref}}^{T_{ut}} C_{p,i} \, dT + \sum_{prod} R_j (-\Delta H_{rxn,j}(T_{ref})) \quad , \; T_{ref} = 298 \text{ K}$$

$$0 = (T_{in} - 298)(10 \cdot 30 + 100 \cdot 25) - (400 - 298)(5 \cdot 30 + 85 \cdot 25 + 10 \cdot 40) + 40000 R$$

$$\Rightarrow T_{in} = 324 \text{ K}$$

David Frisk

(IRV)4



R: $CH_3COCH_3 \longrightarrow CH_2CO + CH_4$
(A) (B) (C)

$$k = \exp\left(34{,}34 - \frac{34222}{T}\right)$$

$$F_A'(1-X) - F_A'(1-X-dX) - r\,dV_r = 0$$

$$F_A'\,dX = r\,dV_r = -k\,c_A\,dV_r \qquad (1)$$

$$\left.\begin{aligned} F_A &= F_A'(1-X) \\ F_B &= F_A'X \\ F_C &= F_A'X \end{aligned}\right\} \qquad C_A = \frac{F_A'(1-X)}{F_A'(1+X)} \cdot \frac{P}{RT}$$

$$F_A'\,dX = k(T)\cdot\frac{(1-X)}{(1+X)}\cdot\frac{P}{RT}\,dV_r$$

Värmebalans: $Q_{in} - Q_{ut} + Q_{reak} + Q_{värm} = 0$

$$Q_{in} = (T - T_{ref})\left(F_A'(1-X)\cdot c_{p,A} + F_A'X\cdot c_{p,B} + F_A'X\,c_{p,C}\right)$$

$$Q_{ut} = (T + dT - T_{ref})\left(F_A'(1-X-dX)\cdot c_{p,A} + F_A'(X+dX)c_{p,B} + F_A'(X+dX)c_{p,C}\right)$$

$$Q_{reak} = F_A'\cdot dX_A\,(-\Delta H_{Rxn})$$

$$Q_{värm} = U\cdot a\cdot(T_a - T)\,dV_r$$

$$\Rightarrow \ldots \Rightarrow F_A'\,dX_A\left(-\Delta H_{Rxn} - (-c_{p,A} + c_{p,B} + c_{p,C})(T - T_{ref})\right) + U\cdot a\cdot(T_a - T)\,dV_r =$$
$$= \left(F_A'c_{p,A} + F_A'X_A(-c_{p,A} + c_{p,B} + c_{p,C})\right)dT$$

Sätt in uttrycket för dV_r (1) i detta uttryck....

$$\Rightarrow \frac{dx_A}{dV_r} = k\,\frac{(1-x_A)}{F_A'(1+x_A)}\cdot\frac{P}{RT} \quad\Rightarrow\quad dx_A = k\cdot\frac{(1-x_A)}{F_A'(1+x_A)}\cdot\frac{P}{RT}\,dV_r$$

Mha ovanstående ekv kan vi ta fram en tabell:

V_r	x	T	ΔX	ΔT
0	0	1035	0,179	..
0,1	0,179	959,7	0,01	..
0,2	0,189	1022,2	0,08	..
0,3	0,271	1015,1	0,05	..
0,4	0,326	1028,2	0,07	..
0,5	0,400	1024,1	0,05	..
⋮	⋱	⋱	⋱	⋱

Och sedan plotta!