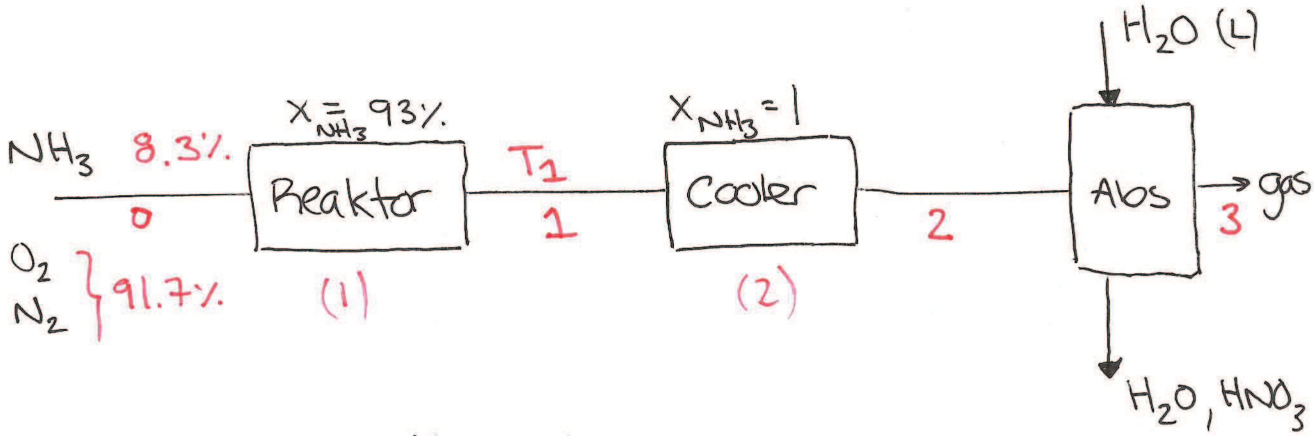
Demoövn. 1

Tis LV1

6.1



(1) $4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

(2) $4NH_3 + 3O_2 \rightarrow 2N_2 + 6H_2O$

Absorption: $4NO + 3O_2 + 2H_2O \rightarrow 4HNO_3 (aq)$

$T_{in} = 600\,°C$

Flow 0

$F_T^0 = 100$ mol/s (basis!)

$F_{NH_3}^0 = 8.3$ mol/s

$F_{O_2}^0 = 91.7 \cdot 0.21 = 19.26$ mol/s

$F_{N_2}^0 = 91.7 \cdot 0.79 = 72.44$ mol/s

luft: 21% O_2, 79% N_2

Flow 1

Frihetsgrad:

system = reaktor

* oberoende variabler:

(1)
- 3 komponenter vid inflödet
- 5 — " — " — utflödet
- 1 reaktion

9 variabler

(2) * Balanser: 5 (= # of components)

(3) * Specifika variabler:

2 oberoende variabler (8.3% NH_3, 91.7% air)

(4) * Hjälp samband (fixed relationship)

1 samband (vi vet X_{NH_3})

(5) * Base of calculation

1 (F_0)

Frihetsgrad: (1) − (2) − (3) − (4) − (5) = 9 − 5 − 2 − 1 − 1 = 0

→ vi har en unik lösning

Massbalans över NH_3

$F^0_{NH_3} - F^1_{NH_3} - R = 0$ vid steady-state!

$$
\begin{array}{lcccc}
 & 4NH_3 & + 5O_2 & \rightarrow 4NO & + 6H_2O \\
\text{initial} & F^0_{NH_3} & F^0_{O_2} & 0 & 0 \\
\text{final} & \underbrace{F^0_{NH_3} - 4r}_{0.07F^0_{NH_3}} & F^0_{O_2} - 5r & 4r & 5r
\end{array}
\Bigg\} \rightarrow R = 4r
$$

$$\rightarrow F^0_{NH_3} - F^1_{NH_3} - R = F^0_{NH_3} - 0.07F^0_{NH_3} - 4r = 0$$

$$0.93\,F^0_{NH_3} = 4r \rightarrow r = \frac{0.93\,F^0_{NH_3}}{4} = 1.93 \text{ mol/s}$$

$$
\begin{cases}
F^1_{NH_3} = 0.58 \text{ mol/s} \\
F^1_{O_2} = 9.61 \text{ mol/s} \\
F^1_{H_2O} = 11.58 \text{ mol/s} \\
F^1_{NO} = 7.72 \text{ mol/s}
\end{cases}
$$

cooler

$$4NH_3 + 3O_2 \longrightarrow 2N_2 + 6H_2O$$

$$F^1_{NH_3} \quad F^1_{O_2} \quad F^0_{N_2} \quad F^1_{H_2O}$$

$$\underbrace{F^1_{NH_3} - 4r}_{=0} \quad F^1_{O_2} - 3r \quad F^0_{N_2} + 2r \quad F^1_{H_2O} + 6r$$

$$r = \frac{F^1_{NH_3}}{4}$$

$$F^2_{NH_3} = 0$$
$$F^2_{O_2} = 9.17 \text{ mol/s}$$
$$F^2_{N_2} = 72.73 \text{ mol/s}$$
$$F^2_{H_2O} = 12.45 \text{ mol/s}$$

$X_{NO} = 95\%$

Absorption

$$4NO + 2H_2O\,(l) + 3O_2 \longrightarrow 4HNO_3\,(aq)$$

$$F^2_{NO} \quad - \quad F^2_{O_2} \quad -$$

$$\underbrace{F^2_{NO} - 4r}_{=0.05 F^2_{NO}} \quad - \quad F^2_{O_2} - 3r \quad -$$

τῃ $X_{NO} = 0.95$ $(1 - X_{NO})$

$$r = \frac{0.95 F^2_{NO}}{4} = \frac{0.95 \cdot \cancel{72.73}\ 7.72}{4} = 1.834 \text{ mol/s}$$

Flow 3

$$F^3_{O_2} = 3.67 \text{ mol/s}$$
$$F^3_{NO_2} = 0.39 \text{ mol/s}$$
$$F^3_{N_2} = 72.73 \text{ mol/s}$$

$$\longrightarrow F^3_{tot} = F^3_{O_2} + F^3_{NO_2} + F^3_{N_2} = 76.79 \text{ mol/s}$$

$$y_{O_2}^{3} = \frac{F_{O_2}^{3}}{F_{tot}^{3}} = 0.048$$

$$y_{N_2}^{3} = 0.947$$

$$y_{NO}^{3} = 0.005$$

T_1 ?

Värmebalans:

$$Q_{in} - Q_{ut} + Q_{reak.} + \underbrace{0}_{\text{ty adiabatiskt!}} = \underbrace{0}_{\text{ty steady-state (ingen ack.)}}$$

$$Q_{in} = \sum_i c_{p_i} F_i^{in} (T_{in} - T_{ref})$$

$$Q_{ut} = \sum_i c_{p_i} F_i^{ut} (T_1 - T_{ref})$$

$$Q_{reac.} = r_i \cdot \Delta H_R(T_{ref})$$

$$\Delta H_R(T_{ref}) = 4\Delta H_{f,NO} + 6\Delta H_{f,H_2O} - 4\Delta H_{f,NH_3}$$

T_{ref} givet vid 25°C

$$\Longrightarrow \Delta H_R(T_{ref}) = -909.6 \text{ kJ/mol}$$

$T_{in} = 600°C$ {givet} så c_p tas vid 600°C

$$\left\{\begin{aligned} c_{p\,NH_3} &= 45.4 \text{ J/mol·K} \\ c_{p\,N_2} &= 30.25 \text{ J/mol·K} \\ c_{p\,O_2} &= 31.87 \text{ J/mol K} \end{aligned}\right\}$$

$$Q_{in} = (600-25)(45.4 F_{NH_3}^{0} + 30.25 F_{N_2}^{0} + 31.87 F_{O_2}^{0}) = 1828.4 \text{ kW}$$

$$Q_{reak.} = -909.6 \cdot 1.93 = -1775.5 \text{ kW}$$

I Q_{ut} är C_p beroende av T_1 som är okänt **ITERERA!**

Gissa $T_1 = 1100\,°C$

$$\left\{ \begin{array}{ll} C_{p\,NH_3} = 50.24 & \\ C_{p\,N_2} = 31.69 & C_{p\,H_2O} = 39.28 \\ C_{p\,O_2} = 33.51 & \\ C_{p\,NO} = 32.8 & \end{array} \right.$$

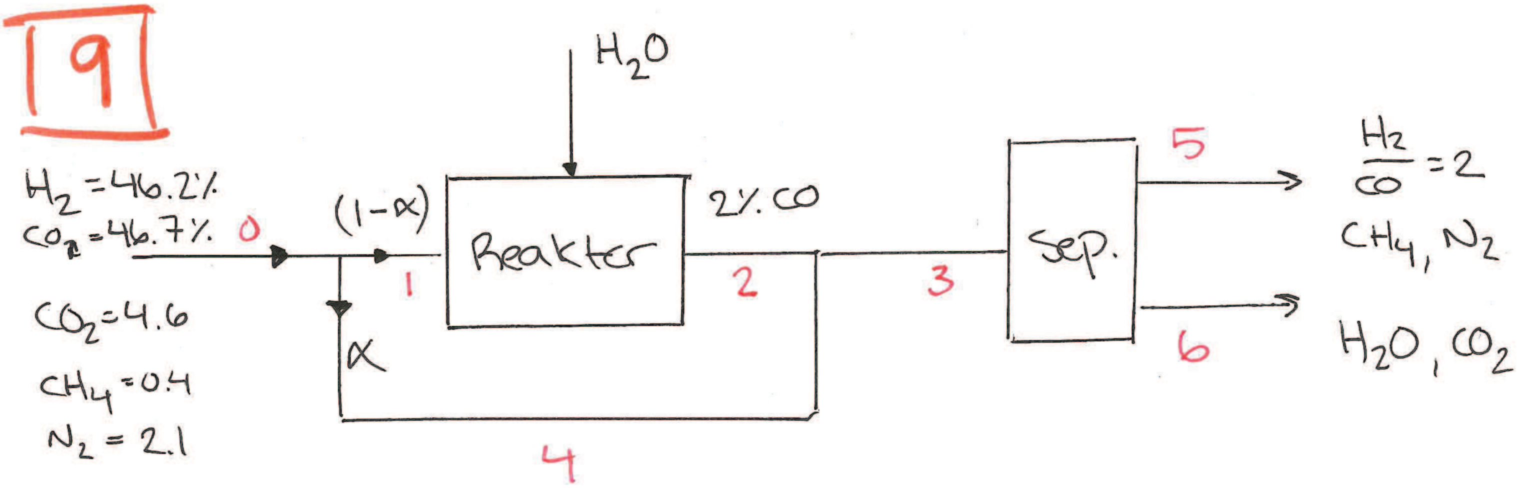
$$Q_{ut} = (T-25)\left(50.24\,F'_{NH_3} + 31.69 \cdot F'_{N_2} + 33.51\,F'_{O_2} + 32.8\,F'_{NO} + 39.28\,F'_{H_2O}\right)$$

$$= 3354.9\,(T_1 - 25)$$

$$1828.4 \cdot 10^3 - 3354.9(T_1 - 25) + 1775.5 \cdot 10^3 = 0$$

$$\longrightarrow T_1 = 1093\,°C$$

9



$$CO_2 + H_2O \longrightarrow H_2 + CO_2$$

a) Sökt: α

$$F_i^1 = F_i^0 (1-\alpha)$$

$$F_{tot}^0 = 100 \text{ mol/s}$$

$$\begin{cases} F_{H_2}^1 = 46.2(1-\alpha) \\ F_{CO}^1 = 46.7(1-\alpha) \\ F_{CH_4}^1 = 0.4(1-\alpha) \\ F_{N_2}^1 = 2.1(1-\alpha) \\ F_{CO_2}^1 = 4.6(1-\alpha) \end{cases}$$

Reaktor $\quad F_{CO}^1 - F_{CO}^2 - R = 0$

Vet att $\quad \dfrac{F_{CO}^2}{F^2 - F_{H_2O}^2} = 0.02$

$$F^2 = F_{CO}^2 + F_{H_2}^2 + F_{CH_4}^2 + F_{N_2}^2 + F_{CO_2}^2 + F_{H_2O}^2$$

$$F^2 = (F_{CO}^1 - \cancel{R}) + (F_{H_2}^1 + \cancel{R}) + F_{CH_4}^1 + F_{N_2}^1 + (F_{CO_2}^1 + R) + F_{H_2O}^2$$

$$F^2 - F_{H_2O}^2 = (1-\alpha)F^0 + R$$

$$0.02 = \frac{F_{CO}^1 - R}{(1-\alpha)F^0 + R}$$

Flow 3

$$F_{CO}^{3} = F_{CO}^{2} + \underbrace{\alpha F_{CO}^{0}}_{F_{CO}^{4}} = \underbrace{F_{CO}^{0}(1-\alpha)}_{F_{CO}^{1}} - R + \alpha F_{CO}^{0} = F_{CO}^{0} - R$$

$$F_{H_2}^{3} = F_{H_2}^{0} + R$$

$$F_{N_2}^{3} = F_{N_2}^{0}$$

$$F_{CH_4}^{3} = F_{CH_4}^{0}$$

$$F_{CO_2}^{3} = F_{CO_2}^{0} + R$$

Flow 5

$$F_{CO_2}^{5} = 0$$

$$F_{CO}^{5} = F_{CO}^{3} = F_{CO}^{0} - R$$

$$F_{N_2}^{5} = F_{N_2}^{0}$$

$$F_{CH_4}^{5} = F_{CH_4}^{0}$$

$$F_{H_2}^{5} = F_{H_2}^{0} + R$$

$$\frac{F_{H_2}^{5}}{F_{CO}^{5}} = 2 = \frac{F_{H_2}^{0} + R}{F_{CO}^{0} - R}$$

$$\longrightarrow R = \frac{47.2}{3} = 15.73 \ \mathrm{mol/s}$$

$$\Longrightarrow \alpha = 0.64$$

b) "Fraction of impurities in flow 5"

$$y_{CH_4+N_2} = \frac{F_{CH_4}^{5} + F_{N_2}^{5}}{F_{CH_4}^{5} + F_{N_2}^{5} + F_{H_2}^{5} + F_{CO}^{5}} = \frac{F_{CH_4}^{0} + F_{N_2}^{0}}{F_{CH_4}^{0} + F_{N_2}^{0} + 2F_{CO}^{5} + F_{CO}^{5}} =$$

$$= \frac{0.4 + 2.1}{0.4 + 2.1 + 3 \cdot 46.7 - 3 \cdot 15.73} = 2.62\,\%$$