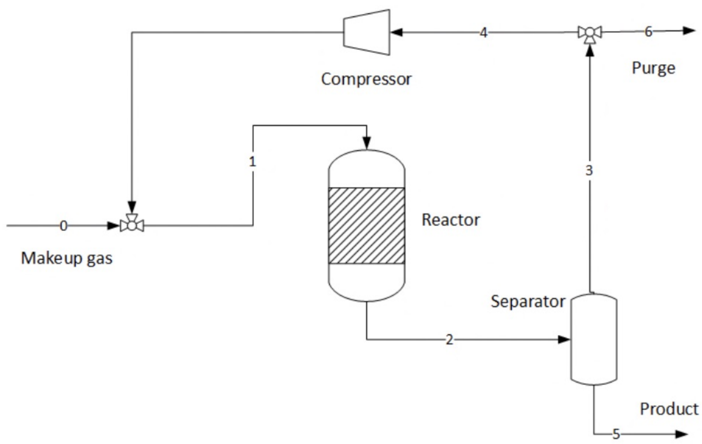
Øving 3

Problem 1

Ammonia synthesis is a gas phase reaction between nitrogen and hydrogen at ca 350 °C and at a pressure of ca 180 bar. $N_2 + 3\,H_2 = 2\,NH_3$



Because there is not complete conversion in the reactor, it is necessary to recycle unconverted gas after ammonia is knocked out. The makeup steam (stream 0) consists of 1 mol% argon (inert) that remains in gas phase. Therefore, it is necessary to purge some of the gas in order to keep the inert concentration at a reasonable level. In this context we only look at the molar flows, therefore the flowsheet does not show that stream 2 is cooled to a temperature where ammonia is condensed and stream 4 is recompressed.

The flow rate of the makeup stream is 1000 kmol/h with a composition of 24 mol% nitrogen, 75 mol% hydrogen and 1 mol% argon. In the separator all argon ends up in the gas phase (over top), and all ammonia ends up in the liquid phase. Furthermore, we assume 99 % of all hydrogen and 98 % of all nitrogen goes over top (on a molar basis). Assume a split flow ratio of 95%, i.e. 5% of stream 3 goes to purge. In the reactor we assume that 30 % of all nitrogen in stream 1 is converted to ammonia.

a) Formulate mol balances for each unit.

b) Calculate molar flow rates for all components and all streams and calculate the stream compositions.

c) Verify that the conservation of mass is fulfilled.

d) Change the split flow ratio in the range from 0.90 to 0.99 and plot the inert concentration of stream 1, recycle ratio and the total purge as function of the split ratio.

a)

La $F_i = \begin{bmatrix} F_{N_2,i} \\ F_{H_2,i} \\ F_{NH_3,i} \\ F_{Ar,i} \end{bmatrix}$

Mixer: $\boxed{F_1 = F_0 + F_4}$

Reactor: Støkiometri

$$N = \begin{bmatrix} -1 \\ -3 \\ 2 \\ 0 \end{bmatrix}, \quad \text{Har } \xi = \underbrace{\begin{bmatrix} \overset{0,3}{\overset{\parallel}{X_{N_2}}} & 0 & 0 & 0 \end{bmatrix}}_{=\mathbb{X}} \cdot F_1$$

$\Rightarrow$ Endring: $N \cdot \mathbb{X} \cdot F_1$

Balanse: $\boxed{F_2 = F_1 + N \cdot \mathbb{X} \cdot F_1 = (\mathbb{I} + N \cdot \mathbb{X}) \cdot F_1}$

Separator

Har $a_k = \begin{bmatrix} 0{,}98 & 0{,}99 & 0 & 1 \end{bmatrix}$

$A = \text{diag}(a_k)$

$$\Rightarrow \boxed{\begin{aligned} F_3 &= A F_2 \\ F_5 &= (\mathbb{I} - A) F_2 = F_2 - F_3 \end{aligned}}$$

Divider: $\boxed{\begin{aligned} F_4 &= 0{,}95 \cdot F_3 \\ F_6 &= 0{,}05 \cdot F_3 \end{aligned}}$

b) Legger massebalansene inn i python

Først: Trenger å finne komposisjonen av $F_1 = F_0 + F_4$ først,

$\Rightarrow$ Må finne F_4

Kombinerer massebalansene:

$$F_4 = 0{,}95 \cdot F_3 = 0{,}95 \cdot A F_2 = 0{,}95 \cdot A(I + NX) \cdot F_1$$

$$F_4 = 0{,}95 \cdot A(I + NX) \cdot (F_0 + F_4)$$

$$\Rightarrow \left(I - \underbrace{\left[0{,}95 \cdot A(I + NX)\right]}_{= M}\right) F_4 = 0{,}95 \cdot A(I + NX) F_0$$

$$\boxed{(I - M) F_4 = M F_0}$$

Får:

```
De molare komponentstrømmene [kmol/h]:
Stream  FN2     FH2     FNH3    FAr     F_tot
---------------------------------------------------
F0      240     750     0       10      1000
F1      689     2802    0       200     3691
F2      482     2182    413         200     3278
F3      473     2160    0       200     2833
F4      449     2052    0       190     2691
F5      10      22      413         0   445
F6      24      108     0       10      142
```

```
Sammensetning av strømmene:
Stream   XN2     XH2     XNH3    XAr
----------------------------------------
F0       0.24    0.75    0.0     0.01
F1       0.19    0.76    0.0     0.05
F2       0.15    0.67    0.13    0.06
F3       0.17    0.76    0.0     0.07
F4       0.17    0.76    0.0     0.07
F5       0.02    0.05    0.93    0.0
F6       0.17    0.76    0.0     0.07
```

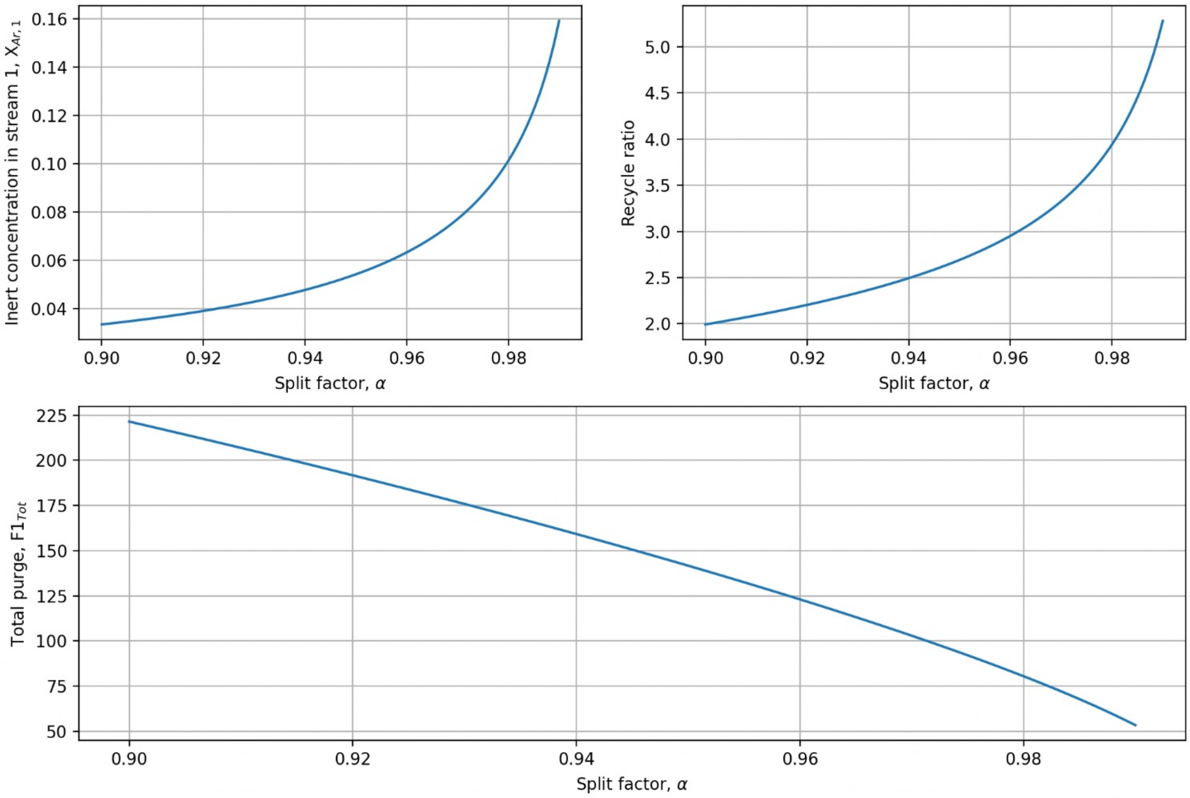
c) Massebevaring: $\dot{m}_0 = \dot{m}_5 + \dot{m}_6$

Sjekker i python

```
Checking mass conservation
----------------------------------------
Mass flow in: 7676.30 kg/h
Mass flow out: 7676.30 kg/h
```

<u>Den er bevart</u>

d) Done in python



b)

1.py > ...

```python
import numpy as np
import matplotlib.pyplot as plt

N2, H2, NH3, Ar = range(4)

N  = np.array([-1.,-3.,2.,0.]).T

F0 = np.array([240.,750.,0.,10.,]).T

A  = np.diag([0.98,0.99,0.,1.])

I = np.eye(4)

alfa = 0.95

XN2 = 0.3

X = np.array([XN2,0.,0.,0.])
```

```python
R = I + np.dot(N,X)

M = alfa*np.dot(A,R)

F4 = np.linalg.solve(I-M,np.dot(M,F0))
F1 = F0 + F4
F2 = np.dot(R,F1)
F3 = np.dot(A,F2)
F5 = np.dot((I-A),F2)
F6 = (1-alfa)*F3
```

=> Print

```
es\lib\python\debugpy\launcher' '60445' '--' 'c:\Users\gvas
[ 689.06115418 2802.4232949     0.           200.        ]
[ 482.34280792 2182.26825614  413.43669251  200.        ]
[ 472.69595177 2160.44557358    0.           200.        ]
[ 449.06115418 2052.4232949     0.           190.        ]
[   9.64685616   21.82268256 413.43669251    0.        ]
[  23.63479759  108.02227868    0.          10.        ]
PS C:\Users\gvass\Documents\Python\TKP4165\Exercise 3>
```

```python
N  = np.array([[-1.],[-3.],[2.],[0.]])
```

```python
X = np.array([[XN2,0.,0.,0.]])
```

Problem 2

In a process 10000 kg/h compressed air is required at 32 atm and 20 °C. Assume air to be an ideal gas with molecular weight 29 g/mol, and as a diatomic gas $\gamma = c_p/c_v = 1.4$. Polytropic efficiency for the compression is assumed to be 75%, $E_p = 0.75$. The air is taken at 20 °C.

a) How will you design the process for air compression. Give reasons for your answer.

b) Calculate the total compression work required and the outlet temperature after the compression.

a) Isoterm kompressjon med mellomkjøling krever mindre arbeid enn adiabatisk kompresjon.

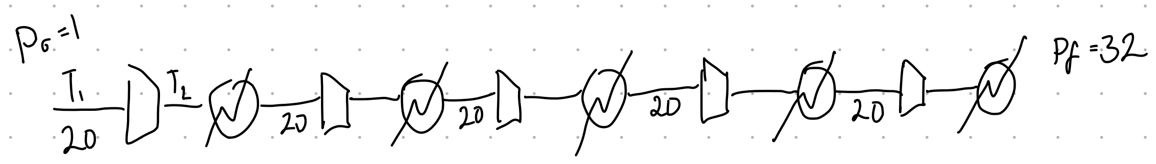
$\approx$ optimal p-forhold : 2

$$\Rightarrow 2^n = \frac{P_f}{P_0} = \frac{32}{1} = 32$$

$$\Rightarrow n = 5$$

Med 5 steg

b)



Reversibelt arbeid for kompresjon

$$W_{rev} = P_1 V_1 \frac{n}{n-1} \cdot \left\{ \left(\frac{P_2}{P_1}\right)^{\frac{n-1}{n}} - 1 \right\}, \quad \frac{P_2}{P_1} = 2, \quad P_1 V_1 = ZRT_1 = RT_1$$

ideal gas

$$m = \frac{\gamma - 1}{\gamma \cdot E_p} = \frac{1{,}4 - 1}{1{,}4 \cdot 0{,}75} = 0{,}381$$

$$n = \frac{1}{1-m} = \frac{1}{1 - 0{,}381} = 1{,}615$$

$$T_1 = 20 + 273 = 293\ K$$

$$\Rightarrow W_{rev} = 8{,}314\ J/mol \cdot K \cdot 293\ K \cdot \frac{1{,}615}{1{,}615-1} \cdot \left\{ 2^{\frac{1{,}615-1}{1{,}615}} - 1 \right\}$$

$$W_{rev} = 1932\ J/mol$$

Denne prosessen skjer 5 ganger per mol gass:

$$W_{rev,tot} = 5 \cdot W_{rev} = 9662\ J/mol$$

$$P = W_{rev} \cdot F \cdot \frac{1}{E_p}$$

power

molar flow

The real work: $W = \frac{W_{rev}}{E_p} = 12883$ J/mol

The moler flow of air:

$$\dot{n} = \frac{\dot{m}}{M} = \frac{10000 \text{ kg/h}}{29 \text{ g/mol}} = 345 \text{ mol/h}$$

Then

$$P = \dot{n} \cdot W = 345 \cdot 12883 \text{ J/h}$$
$$= 4442361 \text{ J/h} \cdot \frac{1 \text{ h}}{3600 \text{ s}}$$
$$\underline{\underline{P = 1234 \text{ kW}}}$$

$T_2 = T_1 \cdot 2^m$

The outlet temperature

$$T_2 = T_1 \cdot \left(\frac{P_2}{P_1}\right)^m = 293\text{K} \cdot 2^{0,381} = 381,5 \text{ K}$$

$$\underline{\underline{T_2 = 108,5 °\text{C}}}$$