

Complete solutions to starred exercises

- Book: *Chemical and energy process engineering*, S. Skogestad, CRC (2008).
- Solutions to the remaining non-starred exercises are only available for instructors.

Exercise 1.1, page 9. *What is a speed of 100 mph (miles per hour) in SI units?*

Solution. $100 \text{ mph} = 100 \cdot 1609.344 / 3600 \text{ m/s} = 44.70 \text{ m/s}$

Exercise 1.3, page 13. *In their design book, Seider et al. (Process design principles, Wiley, 1999) state that a heuristic for an air cooler is that the fan power is 5 hp/(MMBtu/hr). What is the expected fan power (kW) for an air cooler that removes 1 MW of heat?*

Solution.

$1 \text{ Btu/hr} = 0.2931 \text{ W}$

$1 \text{ hp (US)} = 745.7 \text{ W}$

$5 \text{ hp/(MMBtu/hr)} = 5 \cdot 745.7 / 0.2931 \text{ e6 W/W} = 0.0127 \text{ W/W} = 12.7 \text{ kW/MW}$

Conclusion: If you remove 1 MW in a air cooler, then the fan duty is 12.7 kW.

Exercise 1.6, page 26. *Prove that the expression for converting the manufacturer's valve coefficient to SI units is $C_v = C'_v / 41625$.*

Solution

C_v' : manufacturer's valve capacity coefficient,

C_v' = flow [gpm] cold water when $dp=1\text{psi}$

Valve equation (SI units)

$q \text{ [m}^3\text{/s]} = C_v \cdot \sqrt{dp/\rho} = C_v \cdot \sqrt{e5/14.5 \cdot e3}$

where

$dp = 1 \text{ psi} = (1/14.5) \text{ bar} = (e5/14.5) \text{ N/m}^2$

$\rho = 1000 \text{ kg/m}^3$

Convert to gpm

$C_v' = q \text{ [gpm]} = q \text{ [m}^3\text{/s]} / 63.09 \text{ e-6} = C_v \cdot (1/63.09 \text{ e-6}) \cdot \sqrt{100/14.5} = C_v \cdot 41625$

Conclusion: $C_v = C'_v \cdot 63.09 \text{ e}^{-6} \sqrt{14.5 \text{ e}^{-2}} = C'_v / 41625$

Comment:

The KV-value used by valve manufacturers in Europe needs to be divided by 36000. Proof:

K_v = flow [m³/h] cold water when $dp=1\text{bar}$

$dp = 1 \text{ bar} = e5 \text{ N/m}^2$

Valve equation gives under these conditions:

$q \text{ [m}^3\text{/s]} = C_v \cdot \sqrt{dp/\rho} = C_v \cdot \sqrt{e5/e3}$

Convert to m³/h

$K_v = q \text{ [m}^3\text{/h]} = q \text{ [m}^3\text{/s]} \cdot 3600 = C_v \cdot 3600 \cdot \sqrt{100} = C_v \cdot 36000$

Reference: B.L.Liptak (Editor), *Instrument Engineers' Handbook*, 4th Edition, CRC Taylor & Francis and ISA, Volume II (Process control and optimization), p. 1051 (2006)

Exercise 1.7, page 31. *One day, the energy price for electric power is 0.1 \$/kWh. What does this correspond in \$/GJ?*

Solution. $0.1 (\$/\text{kWh}) / (3600 \text{ kJ/kWh}) = 27.8\text{E-}6 \text{ \$/kJ}$

Exercise 1.8, page 31. *One day, the price of oil with density of 0.8 kg/l is 1 \$/l. What does this correspond to in \$/GJ (with water as a gas product)?*

Solution.

$$1 \text{ \$/l} / 0.80 \text{ kg/l} = 1.25 \text{ \$/kg}$$

$$1.25 \text{ \$/kg} / 45\text{e}3 \text{ kJ/kg} = 27.8\text{E-}6 \text{ \$/kJ}$$

Exercise 1.9, page 32. *Given the above energy costs, what is the cost of taking a bath, that is, how much does it cost to heat up 100 l of water from 10 °C to 50 °C with the use of electricity or oil?*

Solution. $Q = 4.18\text{J/K kg} * 40\text{K} * 100 \text{ kg} = 16720 \text{ kJ}$ which corresponds to $16720 * 27.8\text{E-}6 = 0.46$ (that is, 0.46 \$).

Exercise 1.10, page 32. *How much oil [kg] is needed to heat up 100 l of water from 10 °C to 50 °C?*

Solution. 0.372 kg of oil (with water as a gas product): $16720 \text{ kJ} / 45000 \text{ kJ/kg} = 0.372 \text{ kg}$

Exercise 1.11, page 32. *The oil price is one day \$100/barrel. What is this per liter and per gallon?*

Solution. $100 \text{ \$/bbl} / 159 \text{ l/bbl} = 0.63 \text{ \$/l} = 0.63 * 3.785 \text{ \$/gal} = 2.38 \text{ \$/gal}$

Exercise 1.12, page 32. *The price of natural gas varies a lot depending of the location. In October 2005, the gas price varied from \$0.75/million Btu in Saudi-Arabia to \$8/million Btu in West Europe and \$14/million Btu in USA. What does this correspond to in \$/GJ?*

Solution. $0.75 \text{ USD/MBtu} / 1.05505 \text{ kJ/Btu} = 0.71 \text{ \$/GJ}$ (Saudi). Similar: $7.63 \text{ \$/GJ}$ (Europe), $13.25 \text{ \$/GJ}$ (USA)

Exercise 1.13, page 32. *What does a natural gas price of \$/8 million Btu (Western Europe Nov. 2005) correspond to in \$/Sm³?*

Solution. $8\text{e-}6 \text{ USD/Btu} * 42 \text{ e}3 \text{ kJ/Sm}^3 / 1.05505 \text{ kJ/Btu} = 0.32 \text{ \$/Sm}^3$

Exercise 1.14, page 32. *The natural gas production in the Norwegian part of the North Sea was in 2001 about $53 \cdot 10^9 \text{ Sm}^3$ (which was about 2% of world's production of natural gas). What does this correspond to in kg/s and what is the combustion value in GW (assume that the natural gas has molar weight of 18 g/mol and that its heating value (lower heat of combustion) is 42 MJ/Sm^3).*

Solution. $2.237 \text{ e}12 / (365 * 86400) \text{ mol/s} = 70941 \text{ mol/s} = 70941 * 18\text{E-}3 \text{ kg/s} = 1277 \text{ kg/s}$

Combustion: $43 \text{ e}9 \text{ Sm}^3/\text{y} = 43\text{e}9 / (365 * 86400) \text{ Sm}^3/\text{s} = 1363 \text{ Sm}^3/\text{s} = 1363 * 42 \text{ MJ/s} = 70.6 \text{ e}3 \text{ MJ/s} = 70.6 \text{ GW}$

Exercise 1.15, page 32. *In addition to the $53 \cdot 10^9 \text{ Sm}^3$ mentioned above, an additional $34 \cdot 10^9 \text{ Sm}^3$ was reinjected into the ground as pressure support for oil extraction and to avoid flaring. (a) What is the potential value of the reinjected gas, with a gas price of 8 \$/million Btu (Europe, Nov. 2005)? (b) What is its potential value for producing electric energy, if we assume a 50% efficiency for converting it to electric energy and the electricity price is 0.1 \$/kWh.*

Solution

(a) Selling gas: $34\text{e}9 \text{ Sm}^3/\text{y} * 0.32\text{\$/Sm}^3 = 10.9 \text{ E}9 \text{ \$/y}$

(b) combustion: $0.5 * 34 \text{ e}9 \text{ Sm}^3/\text{y} * 42 \text{ E}6 \text{ J/Sm}^3 = 7.14 \text{ e}17 \text{ J/y}$, $1 \text{ kWh} = 1000 \text{ J/s} * 3600 \text{ s} = 3.6 \text{ E}6 \text{ J}$

Value: $7.14 \text{ e}17 \text{ J/y} * 0.1 / 3.6\text{E}6 \text{ \$/J} = 1.98 \text{ e}10 \text{ \$/y} = 19.8 \text{ billion \$/y}$

Exercise 1.16, page 32. *How much CO_2 [Sm^3] is created when we burn 1 l gasoline (assume that the density for gasoline is 0.7 kg/l and that the mole ratio C:H in gasoline is 1:2)?*

Solution. Weight fraction C in "CH₂-gasoline" is $12/(12+2) = 0.857$. 1 l gasoline: $0.857 \cdot 0.7 = 0.60$ kg C or $0.60/12E-3 = 50$ mol or $50/42.292 = 1.182$ Sm³ (this is ISO Sm³)

Exercise 1.17, page 32. *Assume that there are 600 million cars in the world, which annually on average are driven 20000 km with a gasoline consumption of 0.1 l/km. Assume that gasoline has a density of 0.7 g/l and that the lower heat of combustion is 45000 kJ/kg. What is the consumption of gasoline (in l/y and kg/s) and energy (GW) for all these cars?*

Solution. Gasoline consumption pr year: $600e6 \cdot 20e3 \cdot 0.1 = 1.2E12$ l; (seems OK; on the web I found that the world gasoline consumption in 2003 was 1.2 E12 liters $1.2E12 \cdot 0.7$ kg = 8.44E11 kg/y

per s: $8.44E11 / (365 \cdot 86400) = 26636$ kg/s

Energy consumption: 26636 kg/s $\cdot 45$ e6 J/kg = 1.20 E12 J/s

Exercise 1.18, page 32. *The world's yearly energy consumption (2008) corresponds to about 12000 million ton of oil equivalents (toe). What does this correspond to in EJ/y, in kWh/y, and in TW? What is the average energy consumption [kW] per person? (Data: 1 toe corresponds to 42 GJ and there are 6 billion people).*

Solution. The world's energy consumption corresponds to: 12 e9 toe/y $\cdot 42$ e9 J/toe = 5.04 e20 J/y = 504 EJ/y

or 5.04 e20 J/y / 3.6 e6 J/kWh = 1.4 e14 kWh/y

or 1.4 e17 Wh/y / $(365 \cdot 24)$ h/y = 1.60 e13 J/s = 16.0 TW

Per person: 16.0 e12 / $6e9$ = 2667 W = 2.7 kW

Exercise 1.19, page 33. *The world's largest natural gas field is offshore Qatar in the Arabian Gulf. It is given that the total reserves in this field are 900 TCF. How many years of the world's current energy consumption does this correspond to?*

Solution. 1 TCF = 1 terra cubic feet = 10^{12} ft³ = $28.3168 \cdot 10^9$ Sm³. From the rule of thumb this is 28.3 E9 toe. The yearly energy consumption is (2008) is 12 E9 toe, so it is enough for $28.3/12 = 2.35$ years

Exercise 1.20, page 33. Solar cells. *Taking into account that some light is reflected, the earth receives from the sun about 120000 TW which is about 7500 times more than the current worldwide energy consumption (16 TW in 2008). Thus, if we could make effective use of the solar energy, there would no need to worry about the world's energy supply or global warming. The most direct way to utilize the energy from the sun is by solar cells.*

The average solar radiation to the earth is about 240 W/m², but not all this reaches the surface. Assume that the average value in Sahara is 220 W/m². How large area must one cover with solar cells to meet the world's energy demand if the efficiency in a solar cell for conversion to electricity is assumed to be 15%?

Solution. 16 e12 W / $(220 \cdot 0.15)$ W/m² = 4.84 e11 m² = 484 000 km² solar cells

This is about 0.3% of the earth's total land area and about 5% of Sahara. It corresponds to about 80 m² of solar cell panels per person.

Comment. Data from wikipedia: Sahara is the world's largest desert with an area of about 9 065 000 km². Earth total area: 510 072 000 km². Earth land area: 148 940 000 km²

Exercise 1.21, page 33. Electricity price with solar cell. *Let us be a bit conservative, and assume that the radiation from the sun is 100 W/m² on average. What is the resulting energy price (in \$/kWh) if we assume 15% efficiency, a price of solar cells of 1000 \$/m² and linear depreciation over 10 years?*

Solution. Each year: 100 W/m² $\cdot 0.15 \cdot 8600$ h/y = 129 kWh/y,m²

Depreciation over 10 years: 100 \$/m² y.

Electricity price: 100 \$/m² y / 129 kWh/y, m² = 0.78 \$/ kWh

Comment: The electricity production from solar cells is currently (2008) approx. 9000 MW = 0.09 TW, which is only 0.06% of the global energy consumption of 16 TW. The electricity production from solar cells increases by about 50% per year, and as the cost to produce solar cells is reduced (here the process engineer will play an important role!), it is expected the resulting energy price may be less than 0.1 \$/kWh (which is lower than what most people pay today!). The oil company Shell produced in 2001 a study that predicted that solar cells around 2050 would be the planet's most important source of electricity; however, at present, most experts in the energy field find this prediction unlikely.

Exercise 1.22, page 34. *The following data is given for the average energy consumption per day for humans:*

Minimum to survive	900 kcal/d
Student, teacher, office worker	1900 kcal/d
Lumberman, athlete	4500 kcal/d

What is the average energy consumption in Watt?

Solution. 44 W, 92 W, 218 W (thus, a person that sits still produces a heat of about 60 W, i.e. about the equivalent of a light bulb)).

Exercise 1.23, page 34. *How much tortilla chips per day must a student eat to meet his energy demand (given: tortilla chips has an energy content (heat of combustion) of 2150kJ/100g) ?*

Solution. 1900*4.184 kJ/ 21500 kJ/kg = 0.370 kg = 370g

Exercise 1.24, page 34. *The following formula is given for the maximum work a person can perform over a period P:*

$$\dot{W}[\text{W}] = \frac{2500}{\ln P[\text{s}]}$$

What is the maximal work over a period of (a) 2 seconds and (b) 1 hour?

Solution. (a) 3600 W. (b) 305W. **Comment:** Note that work and energy consumption are two different things. Just a fraction of a person's energy consumption from burning food is converted into work in the muscles (maybe 10-30%).

Exercise 1.25, page 34. *What is the average work in Watt when a weight lifter lifts a weight of 200 kg up 1 m in a period of 1 second?*

Solution. $W = mgh = 200 * 1000 * 1 = 2000\text{J}$, i.e 2000W

Exercise 1.26, page 34. *What is the average work in Watt when a person that weighs 80 kg climbs up a 500 m high mountain in a period of one hour? (Note that this is the performed work; the actual energy consumption will be much higher.)*

Solution. $\text{Work} = mgh = 80 * 10 * 500 = 400 \text{e}3$, that is, $400\text{e}3/3600 = 111 \text{ W}$

Exercise 1.27, page 34. *From (6.14), the pump work is $\dot{W}_s = \dot{V} \Delta p$ where $\dot{W}_s [W]$ is the work per unit of time (power), $\dot{V} [m^3/s]$ is the volumetric flow and $\Delta p [N/m^2]$ is the pressure increase. Calculate the work that a human heart performs given the following data:*

- The blood flow for a person at rest is 5 l/min and goes to both the lungs and body (via the two heart chambers).
- The pressure increase for the blood to the lungs is 25 mmHg.
- The pressure increase for the blood to the body is 130 mmHg.

Solution.

5 l/min = 83.3 E-6 m³/s.

25 mmHg = 0.032 bar, $\frac{1}{3}$ 130 mmHg = 0.171 bar

(note that 2 m height is 0.2 bar so some active help from the veins in the legs is required to get it back from the legs.)

Lungs: $W = 83.3 \text{ E-6 m}^3/\text{s} * 0.032 \text{ e5 N/m}^2 = 0.27 \text{ W}$

Body: $W = 83.3 \text{ E-6 m}^3/\text{s} * 0.132 \text{ e5 N/m}^2 = 1.43 \text{ W}$

Sum: 1.7 W

Comment 1. This seems like a low value, but I think it is correct (I checked around on the internet and found estimates around 2-5 W). Also, the work during physical exercise can be about 5 times higher; mainly because of a faster heart rate which increases the flowrate.

Comment 2. The blood pressure varies because the heart works as a piston pump. Normal blood pressures are given as systolic/diastolic gauge pressure [mm Hg]. For example, the value 140/80 (mmHg), means that systolic (peak) pressure is 140 mmHg gauge = 0.187 barg = 1.200 bar, and the diastolic (lower) pressure is 80 mmHg gauge = 0.107 barg = 1.120 bar.

Exercise 1.28, page 35. *A person breathes 20 l/min and the outgoing air is 20 °C warmer than the incoming. (a) What is the heat loss by breath (we do not consider the change in water contents in the air)?*

Solution.

Heat loss by breathing is: $Q = m \text{ CP } dT$ [W]

Data: Density air is 1.19 kg/m³. Heat capacity air is CP=1000 J/kg K.

$m = 20 \text{ l/min} = 20\text{E-3}/60 \text{ m}^3/\text{s} = 0.33 \text{ E-3 m}^3/\text{s}$, i.e., $m = 0.33\text{E-3} * 1.19 \text{ kg/s} = 3.97 \text{ E-4 kg/s}$

$Q = 3.97 \text{ E-4 kg/s} * 1000 \text{ J/kg K} * 20 \text{ K} = 7.9 \text{ J/s} = 7.9 \text{ W}$

Exercise 1.29, page 35. *As discussed in more detail in Chapter 5 on heat exchange, the heat Q [W] transferred from the body to the air through the skin is given by, see equation (5.1),*

$$Q = UA\Delta T$$

where $\Delta T = T_{\text{body}} - T_{\text{air}}$ [K or C] is the temperature difference, A [m²] is the surface area of the body (skin area) and U [W/m² K] is the mean heat transfer coefficient. In this exercise, we assume $U = 5 \text{ W/m}^2 \text{ K}$ and $A = 2 \text{ m}^2$, such that $UA = 10 \text{ W/K}$. The normal body temperature (T_{body}) is 37.0° C.

Problem: At which air temperature will you start sweating when (a) $Q = 100 \text{ W}$ (sitting), (b) $Q = 250 \text{ W}$ (walking) and (c) $Q = 500 \text{ W}$ (jogging).

Solution.

(a) $dT = Q/UA = 100 / 10 = 10 \text{ C}$ ($T_{\text{air}}=27\text{C}$)

(b) $dT = Q/UA = 250 / 10 = 25 \text{ C}$ ($T_{\text{air}}=12\text{C}$)

(c) $dT = Q/UA = 500 / 10 = 50 \text{ C}$ ($T_{\text{air}}=-13\text{C}$)

Exercise 1.30, page 36. *A person stays in a hot climate such that the heat loss, caused by the difference between the body's and air's temperatures, is negligible. How much water must the person evaporate/sweat/perspire in a day given that the average energy consumption is 100 W?*

(Answer. 3.54 kg. This is a lot of sweating! Also note that the person would die if the temperature exceeds 37 °C and the humidity is 100% (such that he or she is unable to sweat). The world can thank us engineers for air conditioning!)

Solution.

Energy consumption 1 day: $Q = 100 \text{ J/s} * 3600 \text{ s/h} * 24 \text{ h/d} = 8.64 \text{ e6 J/d}$

vaporization heat for water is $dH_{\text{vap}} = 2.44\text{e6 J/kg}$.

Evaporates: $m = Q/dH_{\text{vap}} = 8.64 \text{ e6} / 2.44 \text{ e6} = 3.54 \text{ kg/d}$.

Exercise 1.31, page 36. *A sign at the top of the Grand Canyon says that for every hour of hiking in the canyon, you should drink 0.5 to 1 liter of water. Prove this statement by computing the corresponding energy required to evaporate this amount of water.*

Answer. 339W to 678W.

Solution.

$$Q = m \, dH_{\text{vap}} \text{ [W]},$$

where $m = 0.5\text{--}1$ [kg/h] is the amount evaporated
and $dH_{\text{vap}} = 2.44e6$ J/kg is the heat of evaporation for water

$$\text{We get for } m=0.5 \text{ kg/s: } Q = (0.5/3600) \cdot 2.44e6 \text{ W} = 0.5 \cdot 2440/3.6 = 339 \text{ W}$$

$$\text{We get for } m=1 \text{ kg/s: } Q = (1/3600) \cdot 2.44e6 \text{ W} = 2440/3.6 = 678 \text{ W}$$

The corresponding energy consumption is thus 339W-678W which is a reasonable range for hiking in the canyon!

Exercise 1.32, page 36. *In spite of warnings, my daughter Hanne and I did hike from the rim of the Grand Canyon to the river and back in one day. Hanne was wearing a pulse monitor, and when we got back, it estimated that she had used 7000 calories during the hike. How much water does this correspond to if you assume that all the heat loss was due to sweating?*

Answer. 12 kg.

Solution.

First note that when the pulse monitor says "calories" it is actually kcal.

The heat generated during the hike is then

$$Q = 7000 \text{ kcal} = 7000 \cdot 4.184 \text{ kJ} = 29299 \text{ kJ}.$$

Here

$$Q = m \, dH_{\text{vap}} \text{ [kJ]}$$

where

m [kg] is the amount evaporated

$dH_{\text{vap}} = 2.44e6$ J/kg is the heat of evaporation for water

$$\text{We get: } m = 29.299e6 \text{ J} / 2.44e6 \text{ J/kg} = 12 \text{ kg}.$$

This is 12 liters of water.

Comment: She probably did not drink quite this much for the following reasons:

1. The temperature was above 37C for only a part of the day, so she did get some cooling through heat transfer.
2. 7000 cal in 12 hours corresponds to $Q = (7000/12) \cdot 1.16 = 676$ W, which seems high as an average value for the whole day. The pulse monitor may have overestimated Q because Hanne's pulse is normally quite high.

Exercise 2.1, page 46. Perfect membrane unit with cocurrent flow. *By mistake the patient is connected to the membrane unit so that the flow is cocurrent, that is, the two flows enter at the same end. With a perfect membrane we can then assume $c_{B,mem} = c_{D,mem}$ at the exiting end. Assume also here $c_D = 0$ (no urea in entering dialysis fluid).*

(i) *Use the total urea mass balance for the membrane unit to derive an expression for $c_{B,mem}/c_B = (1 - \epsilon)$, where ϵ is the membrane unit's "efficiency" (which was 1 for ideal membrane with countercurrent flow). Note that ϵ should only depend on q_B and q_D .*

(ii) Put this into the dynamic urea mass balance for the patient, and use the given data to calculate the concentration of urea in the blood (c_B) at the end of the treatment ($t=240$ min). (You will find that the urea concentration is about double of that found with countercurrent flow).

Solution.

- (i) total the mass balance for membrane with $c_{D,mem} = c_{B,mem}$ and $c_{D}=0$:
 $q_B c_{B} = q_B c_{B,mem} + q_D c_{B,mem}$
 and we derive $c_{B,mem} = c_{B} * q_B / (q_B + q_D)$, i.e.
 $e = 1 - q_B / (q_B + q_D) = 1 / (1 + q_B / q_D)$
- (ii) Insert into the dynamic mass balance for patient
 $V dc_{B} / dt = q_B c_{B,mem} - q_B c_B$
 where $c_{B,mem} = c_B (1 - e)$. Get
 $V dc_{B} / dt = - e q_B c_B$
 which with constant V , q_B and e has the solution
 $c_{B}(t) = c_{B0} \exp(-e q_B t / V)$.
 Insert numbers: Find $e = 0.625$ and $c_{B}(240\text{min}) = 0.407 c_{B0} = 20.3 \text{ mmol/l}$.

which is about double the 11.8 mmol/l we found with countercurrent flow.

Exercise 2.3, page 52. Mass balance distillation. A 2000 kmol/h feed stream F with 60 mol% methanol and 40 mol% water is separated in a distillation column and gives two products: A "light" methanol product (distillate D) which contains 2 mol% water, and a "heavy" water product (bottoms B) which contains 5 mol% methanol.

- (a) Draw a flow sheet and formulate two mass balances.
 (b) Calculate the amount of methanol product.

Solution:
 (a)
 Total [mol/h]: $F = D + B$
 Methanol [kmol/h]: $z F = y D + x B$,
 where: z, y, x are mole fractions of light component (methanol)

(b) Data: $F=2000$, $z=0.6$, $y=0.98$, $x=0.05$.
 Get: $0.6*2000 = 0.98*D + 0.05*(2000-D)$ Gives $D = 1183$.

Exercise 2.4, page 52. What is the best way to rinse a beaker? We have a 0.5 l beaker where there is a rest of 10 ml water solution with some salt S , with concentration 100 g S/l. We want to rinse the beaker using pure water. After each rinsing there is a rest of 10 ml.

- (a) What is the concentration in the beaker after two rinsings of 200 ml water each?
 (b) What is the concentration in the beaker after four rinsings of 50 ml water each?
 (c) What is the best way to rinse a beaker if we want to use as little water as possible?

Solution

Assume constant density and formulate a total "volume balance" and a mass balance for S [g].
 Initial: 100 gS/l = 0.1 gS/ml.

- (a) After 1st rinsing:
 $0.1 \text{ gS/ml} * 10 \text{ ml} = 1 \text{ g S}$ (S-balance) and 210 ml total (volume balance)
 ie., concentration is $1/210 \text{ g/ml}$ (= 4.76 g/l)
 After 2nd rinsing:
 $1/210 \text{ gS/ml} * 10 \text{ ml} = 1/21 \text{ g S}$ (S-balance) and 210 ml total (volume balance)
 ie., concentration is $(1/21)/210 \text{ g/ml} = 0.227 \text{ g/l}$
- (b) After 1st rinsing: $0.1 * 10 / 60 = 0.1/6 \text{ gS/ml}$
 After 4th rinsing: $0.1 / (6^4) \text{ gS/ml} = 0.077 \text{ gS/l}$

(c) It is better to use several small rinsings.

Exercise 2.5, page 52. Absorption column. *The absorption process in Figure 2.8 uses oil (stream 1) to remove benzene from polluted air (stream 2). (a) How many independent mass balances can be set up? (b) Calculate the amount of oil (stream 1).*

Solution.

Mass balances for 3 components

Oil: $m_1 = 0.99 \text{ m}_3$
 Benzene: $0.04 \text{ m}_2 = 0.001 \text{ m}_4 + 0.01 \text{ m}_3$
 Air: $0.96 \text{ m}_2 = 0.999 \text{ m}_4$

Gven $m_2 = 0.35 \text{ kg/s}$
 Air balance gives $m_4 = 0.3363 \text{ kg/s}$
 Benzene-balance gives $m_3 = 1.3664 \text{ kg/s}$
 Oil balance $m_1 = 1.3527 \text{ kg/s}$
 Check total balance: $m_1 + m_2 = 1.7027$; $m_3 + m_4 = 1.7027$ (OK)

Exercise 2.9, page 55. Mixing volume for ethanol-water. *Use the density data from Example 2.10 to determine the volume when you mix 1 l 96-volume% ethanol and 1 l water at 20 °C. You will find that there is a “loss”, but before you do this, answer subtasks (a)-(d):*

(a) *What is the mass composition of 96 volume% ethanol? (Note that volume% always refers to volumes before mixing!)*

(b) *Use the given density data and to calculate the mass of water and ethanol in 1 l 96 volume% ethanol.*

(c) *We will now look at a mixture of 1 l 96 volume% ethanol and 1 l water. Calculate the composition of the mixture in weight-% and volume-%.*

(d) *Use the given density data and eq. (2.20) to determine the density of your mixture.*

(e) *Finally: What is the volume of your mixture?*

Solution.

Solution:

(a) Basis: 1 l mixture with 0.04 l water and 0.96 l ethanol.
 Mass: $40 \text{ ml} \cdot 0.99823 \text{ g/ml} = 39.9 \text{ g}$ (water) and $960 \text{ ml} \cdot 0.78934 \text{ g/l} = 757.8$ (ethanol),
 that is, 5.01 weight% water and 94.99 weight-% ethanol.

(b) From the given data the density of 96vol%=95wt% is 0.80424 g/l, that is,
 we have $804.24 \cdot 0.00501 \text{ g} = 40.25 \text{ g}$ water and 763.98 g ethanol.
 (Before mixing this corresponds to $40.25 / 0.99823 = 40.32 \text{ ml}$ water
 and $763.98 / 0.78934 = 967.87 \text{ ml}$ ethanol, i.e. total 1008 ml.)
 Conclusion: 40.25 g water and 763.98 g ethanol.

(c) 1 l water = 998.23 g water, that is, we have in total
 $998.23 + 40.25 = 1038.48 \text{ g}$ water and 763.98 g ethanol, i.e. total 1802.46 g,
 so we have 42.39 weight-% ethanol.

Volume fromctions:

1038.48 g water corresponds to $1038.48 \text{ g} / 0.99823 \text{ g/ml} = 1040.32 \text{ ml}$ water
 and 763.98 g ethanol corresponds to $763.98 \text{ g} / 0.78934 \text{ g/ml} = 967.87 \text{ ml}$ ethanol,
 that is, 48.20 volume-%.

Conclusion:

42.39 weight% ethanol and 48.20 volume% ethanol (the answer is somewhat
 more than 48 volume-% because volume is not a conserved quantity, and the
 original 1 l of 96% therefore corresponds to more than 1 l of pure
 water + ethanol).

(d) Interpolation (see comment below) gives that the density is

$$\frac{1}{(w_1/\rho_1)+(w_2/\rho_2)} = \frac{1}{(0.239/0.91384)+(0.761/0.93518)} = 0.92999 \text{ g/ml}$$

which is close to linear interpolation:

$$(1-0.239) \cdot 0.93518 + 0.239 \cdot 0.91384 = 0.9301 \text{ g/l}$$

(e) The volume is $1802.46/0.9300 = 1.938 \text{ l}$.

That is, mixing reduces the volume from 2 l to 1.938 l -- this is because water and ethanol 'like each other'.

Exercise 2.10, page 56. Check of solution. Check that the solution given in the flow sheet in Figure 2.10 satisfies the mass balances

Solution. See equations in Example 2.16 (page 73).

Exercise 2.11, page 61. (a) What is the purge and recycle if $x = 0.5$ and $f = 0.96$?

(b) What is the purge and recycle if $x = 0.5$ and $f = 0.99$?

(c) What is the purge and recycle if the feed contains 99% A and 1% N ($x = 0$, $f = 0.96$)?

Answer. Using the Excel spreadsheet we find: (a) 22.06 mol/s and 529.5 mol/s, (b) 8.59 mol/s and 850.3 mol/s, (c) 10.2 mol/s and 244.6 mol/s.

Exercise 2.12, page 61. (a) What is the recycle (stream 6) if the loss of A is only 1 mol/s? (b) What is the recycle (stream 6) if the feed does not contain any inert (that is, the feed is 100 mol A /s) and we desire 0 loss of A?

Solution. (a) 977.84 mol/s – note that this large stream consists of 75% inert. (b) 255.7 mol/s.

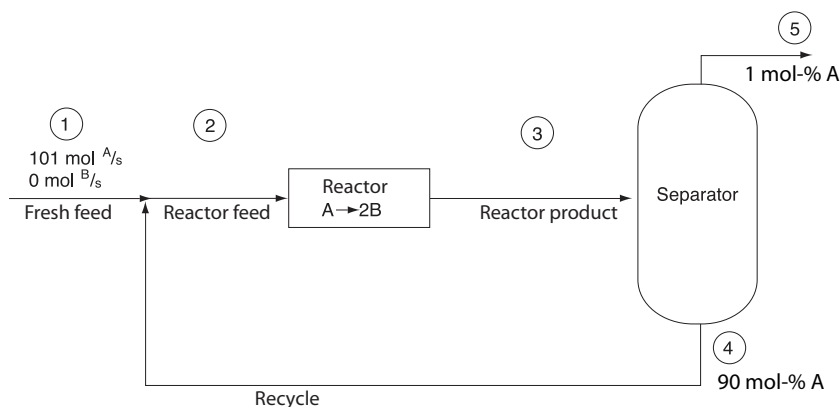


Figure G.1: Flow sheet for exercise process with reactor, separation and recycle

Exercise 2.13, page 62. Consider the process in Figure G.1 where the "heavy" recycle stream (stream 4) is 2000 mol/s. What is the conversion for each pass ($X_A = (n_{A,2} - n_{A,3})/n_{A,2}$)?

Solution. The mass balances for components A and B over the mixing point, reactor and separator give

$$n_{A,2} = n_{A,1} + n_{A,4} \quad [\text{mol A/s}]$$

$$n_{B,2} = n_{B,1} + n_{B,4} \quad [\text{mol B/s}]$$

$$n_{A,3} = n_{A,2} - \xi \quad [\text{mol A/s}]$$

$$n_{B,3} = n_{B,2} + 2\xi \quad [\text{mol B/s}]$$

$$n_{A,4} + n_{A,5} = n_{A,3} \quad [\text{mol A/s}]$$

$$n_{B,4} + n_{B,5} = n_{B,3} \quad [\text{mol B/s}]$$

In addition, we have 5 other pieces of information

$$n_{A,1} = 101 \text{ mol A/s}, \quad n_{B,1} = 0$$

$$\frac{n_{A,5}}{n_{A,5} + n_{B,5}} = 0.01, \quad \frac{n_{A,4}}{n_{A,4} + n_{B,4}} = 0.90$$

together with 1 specification for the recycle,

$$n_{A,4} + n_{B,4} = 2000 \text{ mol A/s}$$

This gives 11 unknowns and 11 equations.

Solution is trivial: Both the composition and flow of stream 4 is known, so we find:

$$n_{A,4} = 1800, n_{B,4} = 200 \text{ mol/s}$$

The reactor feed stream is then (stream 2 = stream 1 + stream 4)

$$n_{A,2} = 1901, n_{B,2} = 200 \text{ molA/s}$$

From the overall balances (not formulated above) and taken into account the stoichiometry ($A \rightarrow 2B$) we must have for the product

$$n_{A,5} = 2, n_{B,5} = 198 \text{ mol/s}$$

(this is the only possibility to get 1% A for the given reaction since the feed is 101 mol A/s). We can the find stream 3 from the mass balance around the separator (stream 3 = stream 4 + stream 5).

$$n_{A,3} = 1802, n_{B,3} = 398 \text{ mol/s}$$

Checking with the material balance for A in the reactor,

$$n_{A,3} = n_{A,2} - \xi \quad [\text{mol A/s}]$$

we then find $\xi = n_{A,2} - n_{A,3} = 1901 - 1802 = 99 \text{ mol A/s}$ (amount of A reacted), which it should be satisfy the overall material balance for A.

Alternatively, we can solve the equations are formulated above. We here choose to use Matlab, but it is trivial by hand.

We write the equations on the form $Ax = b$ where

$$x = [nA1, nB1, nA2, nB2, nA3, nB3, nA4, nB4, nA5, nB5, \xi]$$

and

$$A = \begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \end{bmatrix};$$

```

0  0  -1  0  1  0  0  0  0  0  1  ;
0  0  0  -1  0  1  0  0  0  0  -2  ;
0  0  0  0  -1  0  1  0  1  0  0  ;
0  0  0  0  0  -1  0  1  0  1  0  ;
1  0  0  0  0  0  0  0  0  0  0  ;
0  1  0  0  0  0  0  0  0  0  0  ;
0  0  0  0  0  0  0  0  0.99 -0.01 0  ;
0  0  0  0  0  0  0  0.1 -0.9  0  0  ;
0  0  0  0  0  0  1  1  0  0  0  ]

```

```
b = [0  0  0  0  0  0  101  0  0  0  2000]'
```

```
x=inv(A)*b
```

```
Matlab gives: x = [101 0 1901 200 1802 398 1800 200 2 198 99]'
```

Thus, the conversion is $X_A = (n_{A,2} - n_{A,3})/n_{A,2} = (1901 - 1802)/1901 = 0.0521$.

Exercise 2.16, page 64. Another recycle problem. *2 kg/s of an aqueous solution with 10 weight% of a salt (S) is mixed with a recycle stream. The combined stream is sent to an evaporator where pure water is removed as gas so that the remaining liquid contains 45% S. This is then crystallized and sent to a filter where pure salt (S) is removed while the filtrate (liquid), which contains 20 % S, is recycled.*

(a) *Sketch a flow sheet and formulate the mass balances. Find the amount of recycle.*

(b) *Assume now that the feed in addition contains 1 weight% of another salt (T). The salt T always remains in the water solution (liquid phase), so we purge (drain) 0.04 kg/s of the recycled stream in order to avoid accumulation of T. Otherwise, all the data given above is the same (e.g., the feed is 2 kg/s and contains 10% S, etc.) What is fromction of T in the purge? Calculate the amount recycled.*

Solution.

(a) Let w denote the amount of recycle.

S-balance over the evaporator: $0.2w + 0.2 = 0.45 (w+0.2)$. Get $w=0.44$ kg/s

(b)

$w_1 = \text{feed} = 2$ kg/s

$w_2 = \text{gas(water) leaving evaporator}$;

$w_3 = \text{liquid leaving evaporator=feed crystallizer (45\%S, } x_3 = \text{fraction T)}$

$w_4 = \text{crystal product (pure S)}$

$w_5 = \text{recycled to evaporator (20\%S, } x = \text{fraction T)}$

$w_6 = \text{purge} = 0.02$ kg/s ($x = \text{fraction T}$)

Total: $w_1 = w_2 + w_4 + w_6$, gives $w_2 = 1.98 - w_4$

Total S: $0.1 w_1 = w_4 + 0.2 w_6$, gives $w_4 = 0.1*2 - 0.2*0.04 = 0.192$; ie., $w_2 = 1.788$

Total T: $0.01 w_1 = x * w_6$ gives $x = 0.01*2/0.04 = 0.5$ (fraction T in recirc.)

Total evaporator: $w_1 + w_5 = w_2 + w_3$ gives $2 + w_5 = 1.788 + w_3$

Salt S evaporator: $0.1*2 + 0.2*w_5 = 0.45*w_3$

Solution: $w_3 = 0.6304$, $w_5 = 0.4184$

Exercise 2.17, page 71. Paper machine with fiber recycle (continued).

(a) *Formulate all the mass balances.*

(b) *Find all the stream amounts [kg/s] and fiber fromctions [kg/kg] when we have the following 9 specifications: $A = 100, c_A = 0.1, F = 49, c_F = 0.2, H = 200, c_H = 0.015, L = 20, K = 5000, c_K = 0.002$. What is the "wire retention" $R_W = c_F F / c_D D$?*

Solution.

(a) 14 independent mass balances may be formulated

(e.g. for total mass and fiber for each of the 7 blocks)

(b) Write all the given information on the flow sheet as
[mi (total flow); ci (concentration fiber)].

From the mass balances we can easily obtain the following results
(in the given order):

$$B=A+H=300, \quad c_B=0.043333, \quad C=320, \quad E=C=320, \quad D=5320, \quad G=271, \quad I=71, \quad J=51, \\ c_G=c_H=c_I=0.015, \quad c_E=c_C=0.043328, \quad c_L=0.043250, \quad c_J=0.00392, \quad c_D=0.00449$$

Comment to the solution:

The concept of retention is frequently used when analyzing paper machines.

Retention = portion of supplied component in a stream which is sent to
further processing (product)

The following retentions are of interest:

Retention of fiber in the short circulation:

$$R_K = c_E E / c_D D = 13.865/23.865 = 0.58$$

in the long circulation:

$$R_L = c_F F / c_C C = 9.8 / 13.865 = 0.71$$

Wire retention

$$R_W = c_F F / c_D D = 9.8 / 23.865 = 0.41$$

System retention

$$R = c_F F / c_A A = 9.8 / 10 = 0.98$$

(note that because of recycle the largest streams are about 50 times larger than the feed).

Exercise 2.18, page 75. *The reactor with recycle in Example 2.11 can be described by a set of linear equations $Ax = b$. Use Matlab to find the solution $x = A^{-1}b$, and check that this is consistent with what we have previously found.*

Solution. There are 22 equations; the 19 equations given on page 58 plus 3 given feedflows (for stream 1).

The are 22 unknowns: The 3*7 component flows + the extent of reaction xi (ξ).

Solution using Matlab:

```

naf= 97; nbf= 0; nnf = 3; K=0.3911; x=0 ; f=0.96;

%x =[na1 na2 na3 na4 na5 na6 na7 nb1 nb2 nb3 nb4 nb5 nb6 nb7 nn1 nn2 nn3 nn4 nn5 nn6 nn7 xi]

A = [-1 1 0 0 0 -1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 -1 1 0 0 0 0 -1 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1 1 0 0 0 -1 0 0 ;
      0 -1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 ;
      0 0 0 0 0 0 0 0 0 -1 1 0 0 0 0 0 0 0 0 0 0 0 -1 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1 1 0 0 0 0 0 ;
      0 0 -1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 -1 1 1 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1 1 1 0 0 0 ;
      0 0 0 0 -1 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 -1 1 1 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1 1 1 0 ;
      0 0 -K 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 -1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 -x 0 1 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -1 0 1 0 0 0 0 ;
      0 0 0 0 -f 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 -f 1 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 -f 1 0 0 0 ;
      1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ;
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 ]

```

```

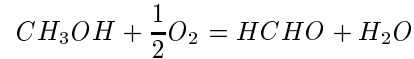
b = [ 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  naf nbf nbf]'
x=inv(A)*b

```

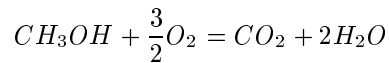
Indeed, this gives the solution shown in the Table on page 57.

We can also solve Exercise 2.11 (page 61) by specifying (a) $x = 0.5$, $f = 0.96$, and (b) $x = 0.5$, $f = 0.99$.

Exercise 3.1, page 84. A reactor is supplied with 1 mol methanol (CH_3OH) and 0.7 mol O_2 . 0.75 mol methanol is converted to the desired product (formaldehyde),



while 0.2 mol methanol is burnt in an undesired side reaction,



(a) Determine the limiting reactant and its conversion. (b) Calculate the extent of reaction for the reactions and the product distribution. (c) Determine the selectivity for methanol to formaldehyde and the yield. (d) Finally, check that $Y = \phi \cdot X$.

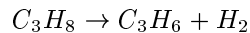
Solution

```

(a) Limiting reactant A is methanol (enough to form 1 mol formaldehyde,
    while we have enough O2 to 1.4 mol).
    Conversion methanol is (0.75+0.2)/1 = 0.95
(b). Extent of reactions are x1=0.75 mol and x2=0.2 mol
    Product from nA = nA0 + nuA1 * x1 + nuA2 * x2
    nmethanol = 1 + (-1) * 0.75 + (-1) * 0.2 = 0.05 mol
    nO2        = 0.7 + (-.5)* 0.75 + (-1.5)*0.2 = 0.025mol
    nformald   = 0 + (+1) * 0.75 + 0 * 0.2 = 0.75 mol
    nH2O       = 0 + (+1) * 0.75 + (+2) * 0.2 = 1.15 mol
    nCO2       = 0 + 0 * 0.75 + (+1) * 0.2 = 0.2 mol
(c) Selectivity for methanol to formaldehyde = converted to desired / total converted
    phi = 0.75/0.95 = 0.7895
    Yield: generated prod/max possible, Y = 0.75/1 = 0.75
(d) Check: Y=phi*X = 0.7895*0.95=0.75, OK!

```

Exercise 3.2, page 85. Reactor with recycle. Propane is de-hydrogenated to propylene in a catalytic reaction



The overall conversion of propane is 95% (for the overall process). The reactor product is separated into two streams: a “light” product with H_2 , C_3H_6 and 0.555% of the C_3H_8 in reactor outlet, and a “heavy” recycle with the remaining C_3H_8 and 5% of the propylene in the reactor product. The recycle is fed back to the reactor.

(a) Draw a flow sheet and perform a quick analytic check if the problem is solvable, for example using Table 2.3.

(b) Calculate the composition of the product.

(c) What is the recycle ratio (amount recycled/amount fresh feed)?

(d) Find the conversion in the reactor.

Solution.

(a) Make flow sheet w/ stream numbers:

Feed 1, Resirc 5, Feed reactor 2, product reactor 3, Product 4.

Quick analysis:

- We know the composition of the feed stream (pure propane assumed), so by assuming a basis, e.g. 100 mol, this is OK.
- For the mixer we need no further information.
- In the reactor we have 1 (independent) reaction, so we need 1 piece of information to find the extent of reaction (and indeed the conversion is given).
- For the separator we be able to determine how each component is split (and this is OK because the composition of the two products are given).
- Conclusion: OK

(b) Basis: 100 mol fresh feed (assumed pure propane).

$NC_3H_8,1 = 100 \text{ mol}$

Let us first look at the overall process

Given overall process conversion = 95%, that is,

$NC_3H_8,4 = 5 \text{ mol}$

Overall propane balance: $Out = In + Generated$
(generated is here negative)

$NC_3H_8,4 = NC_3H_8,1 + (-1) z$

where z [mol] is extent of reaction and (-1) is stoichiometric coeff.

(for C_3H_8 formed by writing the reaction $C_3H_8 = C_3H_6 + H_2$

on the form $0 = -C_3H_8 + C_3H_6 + H_2$.)

We find $z = 100 - 5 = 95 \text{ mol}$

Overall material balances for ethane and hydrogen

(assuming 0 of these in feedstream 1):

$NC_3H_6,4 = z = 95 \text{ mol}$

$NH_2,4 = z = 95 \text{ mol}$

Product:

$NC_3H_8,4 = 5 \text{ mol}$

$NC_3H_6,4 = 95 \text{ mol}$

$NH_2,4 = 95 \text{ mol}$

Total = 195 mol

Composition Product: 2.6% C_3H_8 , 48.7% C_3H_6 and 48.7% H_2

(c) For the separation the following is given

(NOTE: Please read the text carefully!!)

$NC_3H_8,4 = 0.00555 NC_3H_8,3 \rightarrow NC_3H_8,3 = 900.9 \text{ mol}$

$NC_3H_6,5 = 0.05 NC_3H_6,4 \rightarrow NC_3H_6,5 = 4.75 \text{ mol}$

Mass balance propane for separator

$NC_3H_8,3 = NC_3H_8,4 + NC_3H_8,5 \rightarrow NC_3H_8,5 = NC_3H_8,3 - NC_3H_8,4 = 900.9 \text{ mol} - 5 \text{ mol} = 895.9 \text{ mol}$

Get:

Recycle ratio = $N_5/N_1 = 900.65/100 = 9.0065$

(d) Reactor conversion = $(995.9-900.9)/995.9 = 0.0954$.

Comment: Note that the conversion per pass is only 9.55%

but with recycle the overall conversion is 95%

Exercise 3.4, page 91. Propose a reaction set, that is, formulate two independent reactions for Example 3.6. Find N , A , and compute $\text{rank}(N)$, $\text{rank}(A)$ and NA^T .

Solution.

There are many possibilities. Here is one:

rx.1: $CO + 2 H_2 = CH_3OH$

rx.2: $CO + H_2O = CO_2 + H_2$

Components: CO , CO_2 , CH_3OH , H_2 , H_2O

atoms: C , H , O

$N = [-1 \ 0 \ 1 \ -2 \ 0; \ -1 \ 1 \ 0 \ 1 \ -1]$

$A = [1 \ 1 \ 1 \ 0 \ 0; \ 0 \ 0 \ 4 \ 2 \ 2; \ 1 \ 2 \ 1 \ 0 \ 1]$

```

rank(N)=2; rank(A)=3,

>> N*A'
ans =
     0     0     0
     0     0     0

```

Exercise 3.5, page 91. *In each of the following cases you should find the number of independent reactions and propose a reaction set. None of the components are chemically inert.*

(a) H_2 , H_2O , NO and NO_2 .

```

Solution
Nc= 4
Na= 3 (for H, O, N; all of them are independent)
Number of independent reactions Nr=Nc-Na = 4-3 = 1.
Only one possible reaction
NO + H2O = NO2 + H2

```

(b) H_2 , H_2O , O_2 , NO , NO_2 , and N_2 .

```

Solution
Nc= 6
Na= 3 (for H, O, N; all of them are independent)
Number of independent reactions Nr=Nc-Na = 6-3 = 3.
One possible set
rx.1:  H2 + 1/2 O2 = H2O
rx.2:  NO + 1/2 O2 = NO2
rx.3:  N2 + O2 = 2 NO
It is clear that these are independent, since H2O is only in rx.1,
NO2 only in rx. 2, and N2 only in rx.3

```

(c) H_2 , H_2O , O_2 , NO , NO_2 , HNO_3 , NH_3 and N_2 .

```

Solution
Nc= 8
Na= 3 (for H, O, N; all of them are independent)
Number of independent reactions Nr=Nc-Na = 8-3 = 5.

One possible set
(not the simplest one; e.g. may replace rx.4 by N2 + O2 = 2 NO,
but I want to make it a bit difficult):

rx.1:  H2 + 1/2 O2 = H2O
rx.2:  NO + 1/2 O2 = NO2
rx.3:  N2 + 3 H2 = 2 NH3
rx.4:  2NO2 + H2 + O2 = 2HNO3
rx.5:  H2 + N2 + 3O2 = 2HNO3
Are these 5 reactions really independent?
Yes, the stoichiometric matrix N has rank 5; see Matlab code below
H_2, H_2O, O_2, NO, NO_2, HNO_3, NH_3, N_2.
N = [-1  1  -0.5  0  0  0  0  0  0;
      0  0  -0.5  -1  1  0  0  0  0;
     -3  0  0  0  0  0  0  2  -1;
     -1  0  -1  0  -2  2  0  0  0;
     -1  0  -3  0  0  2  0  0  -1]
and we find rank(N)=5.
Further Check: Atom matrix for H, O, N is
% H_2, H_2O, O_2, NO, NO_2, HNO_3, NH_3, N_2.
A = [2  2  0  0  0  1  3  0  0;
      0  0  0  1  1  1  1  2  0;
      0  1  2  1  2  3  0  0  0]

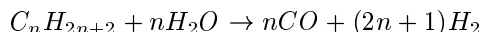
```

Find $\text{rank}(A)=3$ (as expected), and $N'A=0$ (as expected, so stoichiometric matrix is consistent with atom balance)

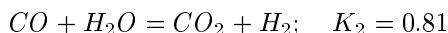
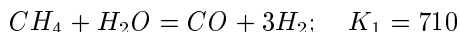
(d) NO , NO_2 , N_2O , N_2 , O_2 , NH_3 and H_2O .

Solution. $\text{nr} = \text{nc} - \text{na} = 7 - 3 = 4$

Exercise 3.6, page 94. Equilibrium for synthesis gas reactor. *The first step in the production of methanol and ammonia is to produce "synthesis gas" consisting of H_2 , CO and CO_2 . This is also a common process for producing hydrogen. Consider a case where the synthesis reactor operates at 21 bar and the feed is a mixture of water vapor and natural gas in the ratio 2.5:1. The natural gas consists of CH_4 (95.5 mol%), C_2H_6 (3.0%), C_3H_8 (0.5%), C_4H_{10} (0.4%) and N_2 (0.6%). The "heavier" hydrocarbons ($n \geq 2$) are assumed to react completely (100% conversion) according to the reactions*



In addition, we have the following equilibrium reactions:



Determine the composition of the product (synthesis gas). (Comment: The temperature at the reactor exit is 880°C . The first reaction is actually not quite in equilibrium and to partly correct this, we have used the thermodynamic equilibrium constant at 864°C).

Answer. Synthesis gas: 11.5% CO , 4.8% CO_2 , 3.9% CH_4 , 52.7% H_2 , 0.1% N_2 , 27.1% H_2O). We get two equations with two unknowns that should be solved numerically, for example with Matlab; see below.

Solution:

Basis: 100 mol natural gas + 250 mol water.

Let us first make a "new" feed consisting of CH_4 , CO , H_2O , H_2 , CO_2 .

Total conversion of C_2H_6 , C_3H_8 , C_4H_{10} by reaction with H_2O to CO and H_2 gives

3 mol C_2H_6 ($n=2$) gives 3mol* (-2 H_2O + 2 CO + 5 H_2)

0.5 mol C_3H_8 ($n=3$) gives 0.5mol* (-3 H_2O + 3 CO + 7 H_2)

0.4 mol C_4H_{10} ($n=4$) gives 0.4mol* (-4 H_2O + 4 CO + 9 H_2)

sum: -9.1 mol H_2O + 9.1mol CO + 22.1 mol H_2

"New feed" is then:

$n_{\text{Och}_4} = 95.5$; $n_{\text{Oco}} = 9.1$; $n_{\text{OH}_2} = 22.1$; $n_{\text{Oh}_2\text{o}} = 240.9$; $n_{\text{On}_2} = 0.6$;

mass balances w/ extent of reactions x_1 and x_2 for the two equilibrium reactions (Matlab code)

---- start matlab ----

% File syngas1.m

% Usage: z = fmins('syngas1',[50 10])

% where [50 10] are start values for the extents of reaction

function z = f(x)

$x_1 = x(1)$; $x_2 = x(2)$;

% feed

$n_{\text{Och}_4} = 95.5$; $n_{\text{Oco}} = 9.1$; $n_{\text{OH}_2} = 22.1$; $n_{\text{Oh}_2\text{o}} = 240.9$; $n_{\text{On}_2} = 0.6$; $n_{\text{Oco}_2} = 0$;

% mass balances

$n_{\text{ch}_4} = n_{\text{Och}_4} - x_1$

$n_{\text{h}_2\text{o}} = n_{\text{Oh}_2\text{o}} - x_1 - x_2$

$n_{\text{co}} = n_{\text{Oco}} + x_1 - x_2$

$n_{\text{h}_2} = n_{\text{OH}_2} + 3*x_1 + x_2$


```

nco2 = n0co2 + x2
nn2 = n0n2;
ntot = nch4+nh2o+nco+nh2+nco2+nn2
% equilibrium
p=21; K1=710; K2=0.81;
Q1a= (nco * nh2^3) / (nch4*nh2o);
Q1 = Q1a * p^2/ntot^2
Q2 = (nco2* nh2) / (nco * nh2o)
z = (Q1/K1-1)^2 + (Q2/K2-1)^2
---- end matlab ----

```

Solution converged (x1 = 75.5, x2=24.9):

```

nch4 = 20.0146          3.86%
nh2o = 140.5490        27.1 %
nco = 59.7197          11.5 %
nh2 = 273.4217        52.7 %
nco2 = 24.8656         4.79%
nn2 = 0.6              0.12%
ntot = 519.1707       100.0 %

```

Exercise 4.2, page 111. Mixing of hot saltwater *2.5 kg/s of hot saltwater with 1 weight% salt and a of temperature 37 °C is to be produced by mixing the following streams: Stream 1 is pure water at 8 °C. Stream 2 contains 10% salt at 80 °C. Stream 3 contains 1% salt at 50 °C. How much is needed of each stream? State clearly all assumptions. (b) How much is needed if stream 3 contains 2% salt?*

Answer. (a) 0.841, 0.093, 1.566 [kg/s]. (b) 0.670, -0.145, 1.965 [kg/s];

Solution

```

(a) Total mass balance: m_1 + m_2 + m_3 = 2.5 [kg/s]
Salt balance: 0 m_1 + 10 m_2 + 2 m_3 = 0.9 \cdot 2.5 [kg salt/s]
energy balance (assume constant cP and neglect heat of mixing)
      8 m_1 + 80 m_2 + 30 m_3 = 37 * 2.5

```

Solve with Matlab

```

A = [1 1 1; 0 10 2; 8 80 50]; b=[2.5; 1*2.5; 37*2.5]; m=inv(A)*b
m' = 0.8405    0.0934    1.5661

```

(b) 2% salt in stream 3

```

A = [1 1 1; 0 10 2; 8 80 50]; b=[2.5; 1*2.5; 37*2.5]; m=inv(A)*b
m' = 0.6703    -0.1449    1.9746

```

The negative sign is, of course, non-physical, because we cannot simply mix streams 1 and 3 and remove stream 2

(as the temperatures and concentrations make this impossible).

Exercise 4.2, page 111. A different process for producing oil-water mixture. *1 kg/s of a product (stream 4), which is a water solution with 30 weight% oil and temperature 20 °C, is produced in a two-step process. In step 1, streams 1 and 2 are mixed and, in step 2, pure water (stream 3) is removed by decanting the water phase (since oil and water naturally form two phases, unless we make an emulsion by strongly mixing the two phases). Stream 1 is pure water at 15 °C and stream 2 is pure oil at 90 °C. Calculate the amount of the four streams. (This looks a lot like exercise 4.3 but note that you here are mixing directly to the desired temperature.)*

Answer. 4.2, 0.3, 3.5, 1 [kg/s].

Solution

Draw a flow sheet!

Overall mass balance: m1 + m2 = m3 + m4

Basis: m3=1 kg/s product.

Mass balance oil gives: $m_2 = 0.3 \cdot 1$
 Energy balance (divide by c_P): $15 m_1 + 90 m_2 = 20 (m_1 + m_2)$, ie. $m_1 = 4.2$
 Overall mass balance gives $m_3 = m_1 + m_2 - m_4 = 4.2 + 0.3 - 1 = 3.5$
 Alternative solution (matlab)

Total mass balance: $m_1 + m_2 = m_3 + 1$ [kg/s]
 component balance oil: $0 m_1 + 1 m_2 = 0 m_3 + 0.3$ [kg/s oil]
 energy balance: $15 m_1 + 90 m_2 = 20 m_3 + 20 \cdot 1$

Matlab:
 $A = [1 \ 1 \ -1; \ 0 \ 1 \ 0; \ 15 \ 90 \ -20]$; $b = [1; \ 0.3; \ 20]$; $m = \text{inv}(A) \cdot b$
 $m' = 4.2000 \quad 0.3000 \quad 3.5000$

Exercise 4.5, page 112. Repeat exercise 4.4 but assume that the decanted stream (stream 3) contains 2 weight% oil. (Answer. 5.6, 0.4, 5.0, 1 [kg/s], that is, 0.1 kg/s oil is lost).

Solution,
 Need to solve the equations simultaneously
 Total mass balance: $m_1 + m_2 = m_3 + 1$ [kg/s]
 component balance oil: $0 m_1 + 1 m_2 = 0.02 m_3 + 0.3$ [kg/s oil]
 energy balance: $15 m_1 + 90 m_2 = 20 m_3 + 20 \cdot 1$
 Matlab:
 $A = [1 \ 1 \ -1; \ 0 \ 1 \ -0.02; \ 15 \ 90 \ -20]$; $b = [1; \ 0.3; \ 20]$; $m = \text{inv}(A) \cdot b$
 $m' = 5.6000 \quad 0.4000 \quad 5.0000$

Exercise 4.7, page 113. We want to find the (final) temperature change when we mix 0.5 kg pure sulfuric acid (H_2SO_4) with 1 kg of pure water to make a 33 weight% sulfuric acid solution. The feeds are at $20^\circ C$. (a) The heat capacity for 33 weight% sulfuric acid is $c_P = 3 \text{ kJ/kg K}$. Use the data on page 417 to show that $\Delta_{\text{mix}} H(20^\circ C) = -217 \text{ kJ/kg solution}$. (b) Find the adiabatic temperature rise. (c) Determine the cooling need to keep the temperature at $20^\circ C$ in a process where we mix 0.5 kg/s pure sulfuric acid (H_2SO_4) with 1 kg/s of pure water.

Solution.

- (a) 1 kg of solution is 333g H_2SO_4 ($=333/98.1=3.39 \text{ mol}$)
 and 667 g H_2O ($=667/18=37.1 \text{ mol}$). $n=37.1/3.39=10.93$.
 From the data we get $dH_{\text{mix}} = -74.7/(1+1.8/10.93)$
 $= -64.1 \text{ kJ/mol } H_2SO_4 = -64.1 \cdot 3.39 = -217.4 \text{ kJ/kg solution}$.
- (b) Energy balance $H_{\text{out}} - H_{\text{in}} = d_1 H + d_2 H = 0$
 sub-processes: 1. mixing at konstant temp: $d_1 H = m_3 \cdot d_{\text{mix}} H$
 2. heat up product: $d_2 H = m_3 \cdot c_{p3} \cdot dT$
 gives $dT = -d_{\text{mix}} H / c_{p3} = 217/3 = 72K$.
- (c) Cooling need: $Q = (-d_{\text{mix}} H) \cdot m = 217.4 \text{ kJ/kg} \cdot 1.5 \text{ kg/s} = 326.1 \text{ kW}$

Exercise 4.9, page 118. A stream of 10 kg/s of methane at 200 bar and $0^\circ C$ is throttled (choked) down to 1 bar. (a) What is the temperature after the choking? (b) How much heat must be supplied to get the temperature back to $0^\circ C$?

Solution:
 (a) Diagram methane: Follow line for constant H: Read off = $-105C$
 (b) at $0C$: $h_1(200\text{bar}) = 345 \text{ kJ/kg}$, $h_2(1 \text{ bar}) = 570 \text{ kJ/kg}$.
 $Q = 10 \text{ kg/s} (570-345) \text{ kJ/kg} = 2250 \text{ kJ/s} = 2.25 \text{ MW}$
 (Answer.) (a) $-105^\circ C$ (b) 2.25 MW.

Exercise 5.1, page 138. A gas stream of 700 mol/s and $C_p = 40 \text{ J/mol K}$ is cooled from 400 °C to 210 °C in a countercurrent heat exchanger by heating liquid water from 100 °C to 350 °C.

(a) Formulate the total energy balance [J/s] and calculate the amount of water, when specific heat capacity for water is 4.18 kJ/kg K.

(b) Calculate UA for the heat exchanger assuming ideal countercurrent flow.

(c) The water flow increases such that the exit temperature of the gas is reduced from 210 °C to 180 °C. Calculate the exit temperature for water and flow of water (you can assume that the inlet temperatures are unchanged, the gas flow is unchanged and UA is constant).

Solution. (a)

$$\underbrace{700 \cdot 40 \cdot 190}_{=5320e3} = m4180 \cdot 250 \quad [J/s]$$

which gives $m=5.09 \text{ [kg/s]}$

(b) $UA = 69910 \text{ W/K}$. $\Delta T_{lm} = (110 - 50) / \ln(110/50) = 76.1 \text{ K}$; $UA = 5320e3/76.1 = 69910$

(c) "Trial and error" gives 304 °C and 7.22 kg/s (to avoid "trial and error" one could use the equations in Section 5.3):

New Q is $700 \cdot 40 \cdot 220 = 6160e3$; which gives $DT_{lm}=88.11$; Trial-and-error gives $DT_2=96K$; i.e. water out 304C; i.e., $m_{water}=6160/4.18 \cdot 204 = 7.22 \text{ kg/s}$

Exercise 5.2, page 139. Comparison of cocurrent flow and countercurrent flows. A hot liquid stream with temperature 37.5 °C is cooled to 20 °C in a heat exchanger where the heat transferred is 73.3 kW. Cooling water with specific heat capacity 4.18 kJ/kg K is used and its temperature goes from 12° C (in) to 17.5° C (out). The overall heat transfer coefficient is $U = 200 \text{ W/m}^2 \text{ K}$. Calculate (a) the amount of cooling water, and the area of the heat exchanger for the cases with (b) countercurrent flow, (c) cocurrent flow and (d) two tube pass with the hot stream on the tube side.

Solution.

(a) In both cases $Q = UA\Delta T_{lm}$. Cooling water $73.3/(4.18 \cdot 5.5) = 3.19 \text{ kg/s}$

(b) Countercurrent, $T_1=37.5-17.5=20$, $T_2=20-12=8$, $T_{lm}=13.1$, $A = 28.0 \text{ m}^2$

(c) Cocurrent $T_1=37.5-12=25.5$, $T_2=20-17.5=2.5$, $T_{lm}=9.9$, $A = 37.0 \text{ m}^2$

(d) Two tube pass (U-turn) with cold stream on tube side (t)

$$Z = T_{sin}-T_{sout} / T_{tout}-T_{tin} = 17.5-12 / 37.5-20 = 5.5/17.5 = 0.3143$$

$$P = T_{tout}-T_{tin} / T_{sin}-T_{tin} = 20-37.5 / 12-37.5 = 17.5/25.5 = 0.6863$$

$$\text{read } F = 0.88 \quad \text{find } A = 28 \text{ m}^2 / 0.88 = 32 \text{ m}^2.$$

Exercise 6.1, page 149. Integrate $W_s^{rev} = \int_{p_1}^{p_2} V dp$ in (6.6) using $pV^\gamma = p_1 V_1^\gamma = \text{constant}$, and show that you get (6.10).

Solution. This is mostly an exercise in integration; note that $\int x^n dx = \frac{1}{n+1} x^{n+1}$. From (A.39) get

$$v = v_1 \left(\frac{p_1}{p} \right)^{\frac{1}{\gamma}} \quad [m^3/mol]$$

which inserted into (6.4) for the shaft work gives

$$w_s^{rev} = \int_{p_1}^{p_2} v dp = p_1^{\frac{1}{\gamma}} v_1 \int_{p_1}^{p_2} p^{-\frac{1}{\gamma}} dp = p_1^{\frac{1}{\gamma}} v_1 \frac{\gamma}{\gamma - 1} \cdot p^{\frac{\gamma-1}{\gamma}} \Big|_{p_1}^{p_2} \quad [J/mol]$$

Here, the last equality holds because $\int a^n = \frac{1}{n+1}a^{n+1}$. We get

$$w_s^{\text{rev}} = \frac{\gamma}{\gamma-1} p_1^{\frac{1}{\gamma}} v_1 \left[p_2^{\frac{\gamma-1}{\gamma}} - p_1^{\frac{\gamma-1}{\gamma}} \right] = \frac{\gamma}{\gamma-1} \underbrace{p_1 v_1}_{RT_1} \left[\left(\frac{p_2}{p_1} \right)^{\frac{\gamma-1}{\gamma}} - 1 \right]$$

and we have derived (6.10).

Exercise 6.2, page 153. 50 mol/s of an ideal gas with heat capacity $C_p = 30$ J/mol K is isothermally compressed (400 K) from 3 bar to 30 bar. The efficiency of the compressor is 0.7. Calculate the required cooling duty.

Solution.

(a) isothermal compression:

$$\begin{aligned} W_s &= n R T \ln p_2/p_1 / \eta \\ &= 50 \text{ mol/s} * 8.314 \text{ J/mol K} * 400 \text{ K} * \ln (30/3) / 0.7 \\ &= 546962 \text{ J/s} = 547 \text{ kW} \end{aligned}$$

Exercise 6.4, page 153. Compressor. In order to produce vacuum and suck off the vapor in Exercise 4.6 (see page 112), a compressor that takes the gas from pressure p_3 to 1 atm is needed.

Data: The vapor pressure of water at 20 °C is $p_3 = 2.337$ kPa, and the compressor has an efficiency of 0.6 (for both adiabatic and isothermal compression). The heat capacity of the gas is 33.6 J/mol K and ideal gas can be assumed. Note that 1 atm is equal to 101.33 kPa and that the amount of compressed is gas 0.0297 kg/s which corresponds to 1.65 mol/s.

Calculate the compression work for both (a) adiabatic and (b) isothermal compression.

Solution

(a)

$$\begin{aligned} \gamma-1/\gamma &= R/c_p = 8.31/33.6 = 0.2473 \\ \text{adiabatic compressionWork: } w_{\text{rev}} &= c_p (T_0-T_3) \\ \text{here } T_0/T_3 &= (p_0/p_3)^{(\gamma-1/\gamma)} = (101.33/2.337)^{0.2473} = 2.5403 \\ \text{i.e., } T_0 &= 2.5403 * 293.15 = 744.7, \text{ dvs} \\ w_{\text{rev}} &= 33.6 * (744.7 - 293.15) = 15172 \text{ J/mol} = 15.2 \text{ kJ/mol} \\ \text{Actual work: } &15.2/0.6 * 1.65 = 41.8 \text{ kW} \\ &\text{(but here the exit temperature is very high)} \end{aligned}$$

(b) isothermal compression:

$$\begin{aligned} w_{\text{rev}} &= RT \ln(p_0/p_3) = 8.31 * 293.15 * \log(101.33/2.337) = 9183 \text{ J/mol} \\ \text{Actual: } &9.183/0.6 * 1.65 = 25.3 \text{ kW.} \end{aligned}$$

Exercise 6.5, page 158. Adiabatic expansion of steam in turbine. 15 t/h of intermediate pressure steam at 30 bar and 450 °C (state 1) is expanded in a (adiabatic) condensing turbine (that is, with cooling at the exit of the turbine, where the vapor is condensed). With maximum cooling at the exit, we are able to reach 0.04 bar (which is the vapor pressure for water at 30 °C). (a) Calculate the work extracted in the turbine, $W_s = H_2 - H_1$, when it is given that the outstream at 0.04 bar (state 2) contains 5% liquid. (b) What is the (adiabatic) efficiency of the turbine (use the expansion from 1 to 2" in Figure 6.12b in order to calculate the reversible work)? Data: HS diagram for water. (Answer. 3.79 MW. 75.2%.)

Solution

(a)

inlet (1) at 30 bar and 450C: $h_1=3350$ kJ/kgexit (2) at 0.04bar/30C and 5% liquid ($x=0.95$): $h_2=2440$ kJ/kgenergy balance (adiabatic process): $W_s = m (h_2 - h_1)$ i.e. $-W_s = (15000/3600)$ kg/s \cdot $(3350-2440)$ kJ/kg = 3791 kJ/s = 3.79 MW

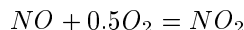
(b) efficiency:

for reversible expansion the entropy would have been constant.

Follow line for constant S from point 1 and down to line for 0.04bar.

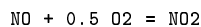
Read of: $h'_2 = 2140$ kJ/kgThat is, for the reversible process: $w_s' = h_1 - h'_2 = 3350-2140 = 1210$ kJ/kgwhereas for the actual process: $w_s = h_1 - h_2 = 3350-2440 = 910$ kJ/kgThe efficiency is then $w_s/w_s' = 910/1210 = 0.752$ (75.2 %).

Exercise 7.3, page 179. NO_x equilibrium. A gas mixture at $940^\circ C$ and 2.5 bar consists of 5% O_2 , 11% NO , 16% H_2O and the rest N_2 . The formation of NO_2 is neglected, and you need to check whether this is reasonable by calculating the ratio (maximum) between NO_2 and NO that one would get if the reaction



was in equilibrium at $940^\circ C$ (use the data on page 416 to determine the equilibrium constant).

Solution. By assuming constant $\Delta_r C_p^\ominus$, we get $K(940^\circ C) = 0.033$ and the ratio is 0.012:



$$\begin{aligned} \text{At } 298K: \quad dhr &= 33 - 90 = -57 \text{ kJ/mol} \\ dgr &= 51 - 87 = -36 \text{ kJ/mol} \\ dcp &= 37 - 30 - 0.5 \cdot 29 = -7.5 \text{ J/mol K} \end{aligned}$$

$$\begin{aligned} \text{At } 940C &= 1213K \\ dhr &= dhr(298) + dcp \cdot dt = -57 - 7.5e-3 \cdot 915 = -63.9 \text{ kJ/mol} \\ dsr_{298} &= (dh-dg)_{298} = -57+36 / 298 = -70.5 \\ dsr &= -70.5 + (-7.5) \ln(1213/298) = -81.0 \text{ J/mol K} \\ dgr &= dhr - 1213 dsr = -63.9 - 1213 \cdot (-81e-3) = + 34.4 \text{ kJ/mol} \\ K \text{ at } 940C &= \exp(-dg/RT) = 0.033 \end{aligned}$$

Assume ideal gas:

$$K = p_{NO_2} / (p_{NO} \cdot p_{O_2}^{0.5})$$

where p is the partial pressure in bar.

If we neglect the formation of NO : $p_{O_2} = 0.05 \cdot 2.5$ bar = 0.125 bar

With this assumption we get:

$$p_{NO_2} / p_{NO} = K \cdot p_{O_2}^{0.5} = 0.033 \cdot 0.125^{0.5} = 0.012$$

That is, we can at the most get 1.2% NO_2 , so it reasonable to neglect its formation

Exercise 7.5, page 182. Test the validity of the simple formula (7.32), by comparing with the following experimental vapor pressure data for water:

$t[^\circ C]$	0	25	50	75	100	120	150	200	250	300	374.14 (T_c)
$p[\text{bar}]$	0.00611	0.03169	0.1235	0.3858	1.013	1.985	4.758	15.53	39.73	85.81	220.9 (p_c)

Also test the validity of the two alternative sets of Antoine constants for water (given in Example 7.13 and Table 7.2).

Solution.

Simple formula is very good over 100C.

1. Antoine formula old: $A = 11.6834$, $B = 3816.44$, $C = -46.13$,
2. Antoine formula new: $A5 = 11.7792$, $B5 = 3885.71$; $C5 = -42.98$;
3. Rule of thumb, $p = (t/100)^4$

t [C]	p1	p2	p3(rule)	pexp
0	0.0059	0.0061	0	0.0061
25.0000	0.0314	0.0318	0.0040	0.0317
50.0000	0.1233	0.1237	0.0633	0.1235
75.0000	0.3856	0.3853	0.3206	0.3858
100.0000	1.0131	1.0104	1.0133	1.0133
120.0000	1.9851	1.9789	2.1011	1.9850
150.0000	4.7624	4.7504	5.1296	4.7580
200.0000	15.5805	15.5839	16.2120	15.5300
250.0000	39.7581	39.9184	39.5801	39.7300
300.0000	84.9322	85.6289	82.0733	85.8100
374.1400	207.4604	210.4410	198.5424	220.9000

```

Generated with Matlab:
A =11.6834, B=3816.44, C=-46.13,
A5=11.7792, B5=3885.71; C5=-42.98; % water H2O
t=[0 25 50 75 100 120 150 200 250 300 374.14]
T=t+273.15, p1=exp(A-B./(T+C)), p2=exp(A5-B5./(T+C5)), p3= ((t/100).^4)*1.01325
pexp= [0.00611 0.03169 0.1235 0.3858 1.013 1.985 4.758 15.53 39.73 85.81 220.9]
[t' p1' p2' p3' pexp']
plot(t,p1,t,p2,t,p3,t,pexp)
plot(t,log(p1),t,log(p2),t,log(p3),t,log(pexp))

```

Exercise 7.6, page 182. Effect of barometric pressure on boiling point.
Assume that the barometric (air) pressure may vary between 960 mbar (low pressure) and 1050 mbar (high pressure). What is the corresponding variation in boiling point for water?

Solution.

```

X1 = fzero(@(T) 0.96-exp(18.3036 - 3816.44/(T-46.13))/750.1,370)
X1 = 371.6477; X2 = 374.1549, delT=X2-X1 = 2.51

```

That is, 2.5 K, which is surprisingly large!

Exercise 7.8, page 195. Bubble and dew point at given temperature. *A hydrocarbon mixture contains 10% propane, 80% hexane and 10% dodecane. (a) Find the bubble point pressure at 300K. (b) Find the dew point pressure at 300K.*

Answer. (a) 1.1585 bar, (b) 0.0018 bar

Solution

```

% Matlab
A7=3.92828; B7= 803.997; C7=-26.11; Tb7=231.02; dvapHb7=19040; % propane C3H8
A2=4.00139; B2=1170.875; C2=-48.833; Tb2=341.88; dvapHb2=28850; % hexane C6H14
A9=4.12285; B9=1639.270; C9=-91.310; Tb9=489.48; dvapHb9=43400; % dodecane C12H26
(a) Bubble pressure
---
T=300; x1=0.1; x2=0.8; x3=0.1
psat1=10^(A7-B7/(T+C7)), psat2=10^(A2-B2/(T+C2)), psat3=10^(A9-B9/(T+C9))
p1=x1*psat1, p2=x2*psat2, p3=x3*psat3
p=p1+p2+p3
y1=p1/p, y2=p2/p, y3=p3/p

```

```

---
Get
p = 1.1585 bar
y1 = 0.8490 y2 = 0.1510 y3 = 1.5993e-005

(b) Dew pressure
T=300; y1=0.1; y2=0.8; y3=0.1
psat1=10^(A7-B7/(T+C7)), psat2=10^(A2-B2/(T+C2)), psat3=10^(A8-B8/(T+C8))
p=1/(y1/psat1 + y2/psat2 + y3/psat3)
x1=y1*p/psat1, x2=y2*p/psat2, x3=y3*p/psat3
---
Get
p = 0.0018 bar (very low because of the heavy component)
x1 = 1.8709e-005 x2 = 0.0067 x3 = 0.9932

```

Exercise 7.9, page 195. Bubble and dew point at given pressure. A hydrocarbon mixture contains 10 mol-% propane, 80% hexane and 10% dodecane. (a) Find the bubble point temperature at 1 bar. (b) Find the dew point temperature at 1 bar.

Solution

```

Matlab
A7=3.92828; B7= 803.997; C7=-26.11; Tb7=231.02; dvapHb7=19040; % propane C3H8
A2=4.00139; B2=1170.875; C2=-48.833; Tb2=341.88; dvapHb2=28850; % hexane C6H14
A9=4.12285; B9=1639.270; C9=-91.310; Tb9=489.48; dvapHb9=43400; % dodecane C12H26

```

```

(a) Bubble point
x1=0.1; x2=0.8; x3=0.1; p=1
T=fzero(@(T) p-x1*10^(A7-B7/(T+C7))-x2*10^(A2-B2/(T+C2))-x3*10^(A8-B8/(T+C8)) , 400)
psat1=10^(A7-B7/(T+C7)); psat2=10^(A2-B2/(T+C2)); psat3=10^(A9-B9/(T+C9));
p1=x1*psat1; p2=x2*psat2; p3=x3*psat3; p=p1+p2+p3, y1=p1/p, y2=p2/p, y3=p3/p

```

```

BUB at 1 bar:
T = 294.7168
y1 = 0.8611 y2 = 0.1389 y3 = 1.1582e-005

```

```

(b) Dew point
y1=0.1; y2=0.8; y3=0.1; p=1
T=fzero(@(T) 1/p-y1/10^(A7-B7/(T+C7))-y2/10^(A2-B2/(T+C2))-y3/10^(A9-B9/(T+C9)) , 400)
psat1=10^(A7-B7/(T+C7)); psat2=10^(A2-B2/(T+C2)); psat3=10^(A9-B9/(T+C9));
x1=y1*p/psat1, x2=y2*p/psat2, x3=y3*p/psat3,

```

```

DEW at p=1 bar:
T = 415.0294 (which is supercritical for propane, so the propane solubility x1 is uncertain)
x1 = 0.0014 x2 = 0.1256 x3 = 0.8730

```

Exercise 7.11, page 195. Flash at given p and T . A feed to a flash tank is 100 mol/s and contains 10% propane, 80% hexane and 10% dodecane. Find the amount of vapor product and the compositions when $T = 350\text{K}$ and $p = 2\text{bar}$.

Solution.

```

Matlab
A7=3.92828; B7= 803.997; C7=-26.11; Tb7=231.02; dvapHb7=19040; % propane C3H8
A2=4.00139; B2=1170.875; C2=-48.833; Tb2=341.88; dvapHb2=28850; % hexane C6H14
A9=4.12285; B9=1639.270; C9=-91.310; Tb9=489.48; dvapHb9=43400; % dodecane C12H26
z1=0.1; xz=0.8; z3=0.1; p=2; T=350;
psat1=10^(A7-B7/(T+C7)); psat2=10^(A2-B2/(T+C2)); psat3=10^(A9-B9/(T+C9));
K1=psat1/p; K2=psat2/p; K3=psat3/p; k1=1/(K1-1); k2=1/(K2-1); k3=1/(K3-1);
Solve Rachford-Rice equation numerically to find a=V/F:
a=fzero(@(a) z1/(k1+a) + z2/(k2+a) + z3/(k3+a) , 0.5)

```

$x_1 = z_1 / (1 + a \cdot (K_1 - 1))$, $x_2 = z_2 / (1 + a \cdot (K_2 - 1))$, $x_3 = z_3 / (1 + a \cdot (K_3 - 1))$
 $y_1 = K_1 \cdot x_1$, $y_2 = K_2 \cdot x_2$, $y_3 = K_3 \cdot x_3$

Solution:

$a = 0.3489$ (so $V = 34.89$ mol/s)
 $x_1 = 0.0181$ $x_2 = 0.2336$ $x_3 = 0.1533$
 $y_1 = 0.2528$ $y_2 = 0.1517$ $y_3 = 4.6842e-004$

Exercise 7.13, page 196. Bubble and dew point calculations. (a) A gas mixture of 15 mol-% benzene, 5 mol-% toluene and the rest nitrogen is compressed isothermally at 100° C until condensation occurs. What will be the composition of the initial condensate?

(b) Calculate the temperature and composition of a vapor in equilibrium with a liquid that is 25 mol-% benzene and 75 mol-% toluene at 1 atm. Is this a bubble-point or a dew-point?

(c) Calculate the temperature and composition of a liquid in equilibrium with a gas mixture containing 15 mol-% benzene, 25 mol-% toluene and the rest nitrogen (which may be considered non-condensable) at 1 atm. Is this a bubble-point or a dew-point?

Solution

1=benzene, 2=toluene, 3=nitrogen

(a) This is a dew point (DEWT). Assume $x_3=0$.

Solution: $p = 6.6439$ bar, $x_1 = 0.5525$ $x_2 = 0.4475$ $x_3 = 0$

% Matlab

$A_{10}=3.98523$; $B_{10}=1184.24$; $C_{10}=-55.578$; $T_{b10}=353.24$; $dvapH_{b11}=30720$; % benzene C6H6
 $A_{11}=4.05043$; $B_{11}=1327.62$; $C_{11}=-55.525$; $T_{b11}=383.79$; $dvapH_{b11}=33180$; % toluene C7H8
 $T=100+273.15$; $y_1=0.15$; $y_2=0.05$; $y_3=0.8$
 $psat1=10^{-(A_{10}-B_{10}/(T+C_{10}))}$, $psat2=10^{-(A_{11}-B_{11}/(T+C_{11}))}$,
 $p=1/(y_1/psat1 + y_2/psat2 + y_3 \cdot 0)$
 $x_1=y_1 \cdot p/psat1$, $x_2=y_2 \cdot p/psat2$, $x_3=0$

(b) This is a bubble point (BUBP).

Solution: $T = 373.3408$, $psat1 = 1.8131$ $psat2 = 0.7466$, $y_1 = 0.4473$ $y_2 = 0.5526$

Matlab:

$x_1=0.25$; $x_2=0.75$; $p=1.01325$
 $T=fzero(@(T) p-x_1 \cdot 10^{-(A_{10}-B_{10}/(T+C_{10}))}-x_2 \cdot 10^{-(A_{11}-B_{11}/(T+C_{11}))}$, 400)
 $psat1=10^{-(A_{10}-B_{10}/(T+C_{10}))}$, $psat2=10^{-(A_{11}-B_{11}/(T+C_{11}))}$,
 $p_1=x_1 \cdot psat1$; $p_2=x_2 \cdot psat2$; $p=p_1+p_2+p_3$, $y_1=p_1/p$, $y_2=p_2/p$,

(c) This is a dew point (DEWP). Assume $x_3=0$ (or $psat3=infinity$).

Solution: $T = 346.7518K$ (73.6C) , $x_1 = 0.1835$ $x_2 = 0.8165$ $x_3 = 0$

Matlab:

$y_1=0.15$; $y_2=0.25$; $y_3=0.6$; $p=1.01325$
 $T=fzero(@(T) 1/p-y_1/10^{-(A_{10}-B_{10}/(T+C_{10}))}-y_2/10^{-(A_{11}-B_{11}/(T+C_{11}))}-y_3 \cdot 0$, 400)
 $psat1=10^{-(A_{10}-B_{10}/(T+C_{10}))}$; $psat2=10^{-(A_{11}-B_{11}/(T+C_{11}))}$;
 $x_1=y_1 \cdot p/psat1$, $x_2=y_2 \cdot p/psat2$, $x_3=0$

Exercise 8.1, page 202. (a) An inventor claims to have produced a machine that takes heat at 200 ° C and removes 50% of it as work. Is this possible? (Hint: Calculate the theoretical cooling temperature.)

(b) Is a reversible process in equilibrium? What is the entropy change for a reversible process? (Hint: Calculate the theoretical cooling temperature.)

Solution. (a) No, Carnot factor = $1 - T_0/T = 1 - T_0/473 = 0.5$ implies that $T_0 = 0.5 \cdot 473K = 236.5$ K (subambient)

(b) Yes, a reversible process goes through a set of equilibrium states. Entropy change is zero (for system + surroundings)

Exercise 8.4, page 222. *In the above example, the exhaust gas was separated into two gas products (pure CO₂ and the remaining exhaust gas).*

(a) *Find the ideal work for separating the exhaust gas into four pure gas components (CO₂, N₂, O₂, H₂O) (you should find that the work is about 5 times larger in this case).*

(b) *Find the ideal work for separating the exhaust gas into two gas products (pure CO₂ and a N₂/O₂-mixture) plus pure liquid water. (Note that $W_s^{\text{id}} = \Delta H - T_0 \Delta S$, and since $\Delta H < 0$ for this process because of the condensation of water, you should find that you actually can extract work in this case, but this does not seem very realistic in practice...)*

Solution:
 (a) For gas components:
 $-T_0 R (62.5 \ln 0.041 + 1177 \ln 0.767 + 169 \ln 0.110 + 125 \ln 0.081) = 2.97 \text{ MJ}$
 (b) Three fromctions:
 $\Delta H = 125 \text{ mol} * (-40) \text{ kJ/mol} = -5 \text{ MJ}$ (condensation of water)
 $W_{\text{sid}} = dH - T_0 dS = 125 * 40 \text{ e}3 - T_0 R (62.5 \ln 0.041 + 1346 \ln 0.877 + 125 \ln 0.081)$
 $= -5 \text{ MJ} + 1.71 \text{ MJ} = -3.3 \text{ MJ}$
 Note: An amine wash may take out water(1) so it may in theory generate work!
 -- not likely in practice though... :-)

Exercise 10.3, page 270. *An irreversible liquid-phase reaction $A \rightarrow P$ with reaction rate $(-r_A) = kc_A$ takes place in an isothermal ideal continuous stirred tank reactor (CSTR). The density of the liquid can be assumed constant. The volumetric feed rate is 0.1 m³/min, $c_{A0} = 10 \text{ mol/m}^3$ and the reactor volume is 1m³. The temperature is 50 °C and the reaction rate constant at this temperature is 0.003 s⁻¹.*

(a) *What is the conversion in the reactor?*

(b) *The reaction is instead performed in an isothermal plug flow reactor (PFR) with volume 1 m³. What is the conversion now?*

Solution. (a) 0.643. (b) 0.835. Details MISSING

Exercise 10.5, page 270. *Component A dimerizes in an irreversible liquid-phase reaction $2A \rightarrow P$ with reaction rate $r_P = kc_A^2$. The reaction takes place in a continuous stirred tank reactor (CSTR). The volumetric feed rate is 0.1 m³/s and $c_{A0} = 2 \text{ mol/l}$. The rate constant at 363 K is $k = 0.0003 \text{ l/mol s}$. The activation energy is $E = 96 \text{ kJ/mol}$.*

(a) *The reactor operates at 386 K. Find the rate constant at this temperature.*

(b) *Formulate the mass balance for component A.*

(c) *Given that the conversion of A is 66%, what is the reactor volume?*

(d) *Will the conversion increase if you replace the CSTR reactor with a plug flow reactor (PFR) with the same volume (give your reasons)?*

Solution:
 (a) From Arrhenius-equation find $k_{386} = 0.0020 \text{ mol/l,s}$
 (b) Mass balance for A: $n_{0a} = n_a - 2k c_a^2 V \text{ [mol/s]}$;
 (c) $n_{0a} = v * c_{0a}$, $n_a = v * c_a$, where v is volumetric flow rate [m³/s]
 Introduce conversion, $n_a = n_{0a} (1 - x_a)$. Find $V = 71.4 \text{ m}^3$
 (d) Yes. PFR needs a smaller volume since reaction order (=2) is positive

Exercise 10.6, page 270. (a) *The irreversible liquid-phase reaction $A \rightarrow P$ with reaction rate $-r_A = kc_A$ takes place in an isothermal batch reactor with constant*

volume. After five minutes, the conversion of A is 30%. How long does it take before the conversion is 50%?

Data: $T = 323 \text{ K}$, $c_{A0} = 1 \text{ mol/l}$, $V_{\text{batch}} = 100 \text{ l}$.

(b) The reaction is instead performed in a plug flow reactor (PFR) with volume 1 m^3 and feed rate $0.1 \text{ m}^3/\text{min}$. What is the conversion now?

(Answer. (a) $k = 0.0713 \text{ min}^{-1}$ gives $t = 9.72 \text{ min}$. (b) Reaction time 10 min gives 51%.)

Solution. MISSING Need to add

Exercise 11.2, page 299. Evaporator Take another look at the evaporator in Example 11.2. What is the time constant for the temperature response?

Answer. $\tau = mc_{pL}/wc_{pV}$ which is larger than the residence time since $c_{pL} > c_{pV}$; for water we have that $c_{pL}/c_{pV} \approx 2.2$.

Exercise A.1, page 328. Show that 1 liter of water contains 55.5 mol of water molecules.

Solution. 1 liter = 1 kg = $1/18.015 \text{ e-3 mol} = 55.5 \text{ mol}$

Exercise A.2, page 331. The boiling point (T_b) depends on pressure, and we want to use (A.3) to find how the boiling point of water depends on elevation.

(a) Use the Antoine vapor pressure formula from Example 7.13 (page 181) to derive an expression for how the boiling temperature of water depends on elevation h .

(b) Show that the boiling point of water drops about 0.35K per 100 m.

(c) What is the boiling point of water at Mount Everest (8850m) ?

Solution. (a) $T_b[\text{K}] = 46.13 + 3816.44/(11.6703 + 1.25 \cdot 10^{-4}h[\text{m}])$. (b) $dT_b/dh = -0.0035 \text{ K/m}$. (c) 344.8 K (71.7 °C). (which means that boiling an egg will take longer time at higher elevations)

Exercise A.3 (page 341). The experimental compressibility factor of saturated ammonia at $T = 325 \text{ K}$ and $p = 21.2 \text{ bar}$ is $z = 0.81$. Check this using (a) the thermodynamic diagram for ammonia on page 419 (you will need to extrapolate outside of the diagram), (b) the generalized compressibility diagram in Figure A.3, (c) van where Waals equation, and (d) the Redlich-Kwong equation. Data: $T_c = 405.7\text{K}$, $p_c = 111.3 \text{ bar}$.

Answer. (b) $z = 0.84$, (c) $z = 0.894$, (d) $z = 0.864$.

Solution

$\text{Tr}=0.801$, $\text{pr}=0.188$.

ideal gas. $\text{Vid} = \text{RT}/p = 8.31 \cdot 325 / 21.2 \text{E}5 = 0.00127 \text{ m}^3/\text{mol}$.

(a) $T=51.85\text{C}$. This is outside the diagram, but by extrapolation we get approx.
 $v=0.06 \text{ m}^3/\text{kg} = 0.06 \cdot 17.03 \text{E-}3 = 0.00102 \text{ m}^3/\text{mol}$, i.e., $z = pV/\text{RT} = \text{V}/\text{Vid}=0.80$.

(b) $z=0.84$

(c) Van where Waals. $a = 0.42188 \text{ R}^2 \text{ Tc}^2/p_c = 0.431$, $b = 0.125 \text{ R Tc}/p_c = 3.79\text{E-}5$

Het cubic equation in V. Solution Matlab:

$b=3.79\text{e-}5$; $a=0.431$; $p=21.2\text{e}5$; $R=8.31$; $T=325$;

$C(1)=p$, $C(2)=-(b \cdot p + R \cdot T)$; $C(3)=a$; $C(4)=-a \cdot b$; $\text{roots}(C)$

Gives $V = 1.139\text{E-}3 \text{ m}^3/\text{mol}$, i.e., $z = pV/\text{RT} = \text{V}/\text{Vid}=1.139\text{e-}3/1.274\text{e-}3 = 0.894$

(d) RK. Solution: From (A.12) find $ac=0.437$ and $b=2.63\text{e-}5$.

Solution of cubic equation with Matlab gives (see below):

$V=1.101\text{E-}3 \text{ m}^3/\text{mol}$ and we have $z = pV/\text{RT} = 0.864$.

Matlab:
 $b=2.63e-5$; $ac=0.437$; $p=21.2e5$; $R=8.31$; $T=325$; $Tc=405.7$; $a = ac/\sqrt{T/Tc}$;
 $C(1)=p$; $C(2)= - R*T$; $C(3)=(a-p*b*b-b*R*T)$; $C(4)=-a*b$; $roots(C)$

Exercise A.5, page 359. Heat of vaporization for water. Given for water: $C_p(l) = 75.4 \text{ J/mol K}$ and $C_p(g) = 33.6 \text{ J/mole K}$ (both assumed constant) and $\Delta_{\text{vap}}H = 40.6 \text{ kJ/mol}$ at 100°C and 1 atm . (a) Use the result from Example A.15 to calculate the heat of vaporization for water at 25°C .

(b) The critical temperature for water is 647.3 K . Compare this with the value of T that gives $\Delta_{\text{vap}}H(T) = 0$ using the simplified expression where we assume constant heat capacities.

Solution. (a) Heat of vaporization as function of temperature is:

$$40600 + (75.4-33.6) (373.15-T) = 40600 + 41.8 (373.15-T)$$

That is, at 25°C : $40600 + 41.8 * 75 = 43735$ (which close to the correct value of 44.0 kJ/mol .)

(b) 1344 K (so it is obvious that the assumption of constant heat capacities and ignoring pressure effects is not suitable near the critical point.)

Exercise A.6, page 364. The (higher) heat of combustion for methyl formate (HCOOCH_3) (l) to H_2O (l) at 25°C is, in an old reference book given as 234.1 kcal/mol . (a) Calculate the standard heat of formation for methyl formate. (b) Which value do you find in a reference book (e.g. *SI Chemical Data*)?

Solution. (a) -379.2 kJ/mol . (b) -387 kJ/mol .

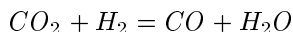
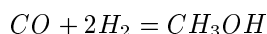
Exercise E.1, page 411. Methanol is removed from a gas stream, where it is mixed with an inert gas. This takes place by decomposing the methanol in water in a absorptions column (see Figure 1.4). 100 mol/s of a gas stream with 7 mol\% methanol is treated with a liquid stream with 500 mol/s of pure water such that the cleansed gas stream is free of methanol. The inert gas is not loosen in water.

(a) Formulate the three independent mass balances.

(b) Find the amount and composition of the two product streams.

Solution. 507 mol/s liquid out

Exercise E.6, page 412. In a continuous methanol reactor that operates at 100 bar , the following gas phase reactions take place



(the last is a “shift reaction”).

(a) Introduce the extent of reaction ξ_j for the reactions and formulate the mass balances (you can denote the feed with N^0 and the product with N).

(b) The feed is 5000 mol/s and has the following composition ($i \text{ mol\%}$)

$\text{CO} : 7.0\%$

$\text{CO}_2 : 2.0\%$

$\text{H}_2 : 75.0\%$

$$CH_4 : 16.0\%$$

Find the product composition when 2/3 of the supplied CO and CO₂ reacts to methanol and it is generated 40 mol/s of water (**Answer.** 90 mol/s CO).

(c) Formulate the energy balance. The feed is at 150 °C and the product at 270 °C. How much cooling is needed in the reactor? (Use the component data given on page 416) (**Answer.** 10.5 MW)

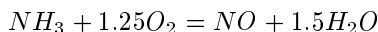
(d) What is the product composition if it is generated 300 mol/s methanol and the shift reaction is in equilibrium at 270 °C? Assume that the equilibrium constant for the shift reaction is $K = 0.016$. (**Answer.** 86.5 mol/s CO)

(e) Find the equilibrium constant for the first reaction at 270 °C and check how close it is from the equilibrium in item (d).

Solution. $K = 0.00076$ and $Q = 0.00069$, i.e. almost equilibrium.

Exercise E.7, page 412. Combustion of ammonia to NO

Nitric acid is produced usually in a process where ammonia is burnt with air (with platinum as catalyst) and generates nitric gases that are cooled and absorbed in water. We consider the first part of the process (see Figure E.2), where we assume that ammonia burns completely following the gas phase reaction:



Data: Assume that the air contains 21% oxygen. The standard heat of reaction is $\Delta_r H^\ominus(298K) = -227$ kJ/mol and $\Delta_r H^\ominus(1213K) = -223$ kJ/mol. Assume constant mean heat capacities:

$$C_p(NH_3)(g) = 37 \text{ J/K mol (up to } 230 \text{ }^\circ\text{C)}; = 54 \text{ J/K mol (} 230 \text{ }^\circ\text{C to } 940 \text{ }^\circ\text{C)}$$

$$C_p(\text{luf}) (g) = 29 \text{ J/K mol (up to } 230 \text{ }^\circ\text{C)}; = 32 \text{ J/K mol (} 230 \text{ }^\circ\text{C to } 940 \text{ }^\circ\text{C)}$$

(a) The reactor feed is a gas mixture of air and ammonia. Introduce the extent of reaction of the reaction and formulate the mass balance of the reactor.

(b) Find the composition of the reactor feed and reactor product when it is assumed adiabatic reactor.

(c) Find the efficiency of the compressor from the data given in the figure.

(d) We neglected the formation of NO₂. To see that this is a reasonable assumption, find the ratio between NO₂ and NO, which could be theoretically obtained if the reaction



was in equilibrium at 940 °C and 2.5 bar (use SI Chemical Data to find the equilibrium constant).

Answer. (b) Feed: 11% NH₃ and 89% air. Product: 11% NO, 16% H₂O, 5% O₂, 68% N₂. (c) 67.9%. (d) $K = 0.033$; NO₂/NO = 0.012.

Solution:

(a) mass balances for the reactor (Out = In + Generated by reaction) [mol/s]

n = reactor product

n0 = reactor feed

X = extent of reaction for the reaction [mol/s].

$$n_{NH_3} = n_{0NH_3} - X$$

$$n_{O_2} = n_{0O_2} - 1.25 X$$

$$n_{NO} = \quad \quad + X \quad \quad (\text{assumer no NO in the feed})$$

$n_{H_2O} = \quad + 1.5 X$ (assumer no H_2O in the feed)
 $n_{N_2} = n_{O_2}$
 Totalt: $n = n_0 + 0.25X$

Note: Since all ammonia combusts, we get $n_{NH_3}=0$, i.e., $X=n_{ONH_3}$.

(b) Assume adiabatic conditions in reactor.
 Energy balance for adiabatic reactor: $H_{out}=H_{in}$.

Basis: $n_0=1$ mole feed with n_{ONH_3} mol ammonia

Evaluate $H_{out}-H_{in}$ by considering

- Heating of feed from 230C to 940C
 $[54 \cdot n_{ONH_3} + 32 \cdot (1 - n_{ONH_3})] \cdot (940 - 230)$ [J]
 where 54 and 32 is C_p -value for component i [J/mole K]
- Reaction at 940C
 $X \cdot dH_r = n_{ONH_3} \cdot (-223e3)$ [J]

Set sum equal to 0 and find that $n_{ONH_3} = 710 \cdot 32 / (223e3 - 710 \cdot 22) = 0.110$
 i.e., the feed mixture is 11% ammonia and 89% air.

The feed is then (basis $n_0=1$ mole)

NH_3 : 0.11 mole
 O_2 : $0.89 \cdot 0.21 = 0.187$ mol
 N_2 : $0.89 \cdot 0.79 = 0.703$ mol

Product is then (extent of reaction for the reaction is 0.11 mole)

NH_3 : 0 mol
 O_2 : $0.187 - 0.11 \cdot 1.25 = 0.050$ mol
 NO : 0.11 mole
 H_2O : $0.11 \cdot 1.5 = 0.165$ mol
 N_2 : 0.703 mol
 Totalt: 1.028 mol

(c) Use that the feed is 11% ammonia and 89% air.

Energy balance ($H_{out}=H_{in}$) for mixing point gives:

$0.11 \cdot 37 \cdot (230 - (-15)) = 0.89 \cdot 32 \cdot (T_6 - 230)$
 V_i finner at $(T_6 - 230) = 35K$ i.e., $T_6 = 265C = 538K$,
 where T_6 is temperature after compression.

Supplied work in compression equals enthalpy difference for air from
 $T_5 = 100C$ to $T_6 = 265C$, i.e., $W_s = C_p(T_6 - T_5) = 29 \cdot 165 = 4785$ J/mole.

For a adiabatic reversible compression we would have

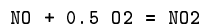
$$(T_6^{rev}/T_5) = (p_6/p_5)^{(R/C_p)} = 2.5^{(8.31/29)} = 1.300$$

which with $T_5 = 373K$ gives $T_6^{rev} = 485K$, i.e., $W_{srev} = C_p(T_6^{rev} - T_5) = 29 \cdot 112 = 3248$ J/mol

i.e., adiabatic efficiency is

$$3248/4785 = 0.679$$

(d) Consider reaction



At 298K: $dH_r = 33 - 90 = -57$ kJ/mol
 $dG_r = 51 - 87 = -36$ kJ/mol
 $dC_p = 37 - 30 - 0.5 \cdot 29 = -7.5$ J/mole K

At 940C = 1213K

$dH_r = dH_r(298) + dC_p \cdot dt = -57 - 7.5e-3 \cdot 915 = -63.9$ kJ/mol
 $dS_r(298) = (dH - dG) / 298 = -57 + 36 / 298 = -70.5$
 $dS_r = -70.5 + (-7.5) \ln(1213/298) = -81.0$ J/mol K
 $dG_r = dH_r - 1213 dS_r = -63.9 - 1213 \cdot (-81e-3) = + 34.4$ kJ/mol
 K at 940C = $\exp(-dG/RT) = 0.033$

(Comment: Using C1-C1, where we assume $dC_p=0$ (i.e., dH_r constant), gives $K_{298}=2.06 \text{ e}6$ and $K_{1213}=0.059$, i.e., ca. a factor 2 different)

We have $K = p_{\text{NO}_2} / (p_{\text{NO}} * P_{\text{O}_2}^{0.5})$ where p is partial pressure in bar.
The partial pressure of oxygen in the product is $(0.050/1.028)*2.5 \text{ bar} = 0.122 \text{ bar}$
(when formation of NO_2 is negligible).

We then find that the ratio between amount of NO_2 and NO equals

$p_{\text{NO}_2} / p_{\text{NO}} = K * P_{\text{O}_2}^{0.5} = 0.033 * 0.122^{0.5} = 0.012$
which is small, i.e., it is reasonable to neglect the formation of NO_2 .

Comment.

This shows how I computed the heat of reaction for the main reaction.

Component data from SI Chemical Data:

no2,	dhf=+33,	dgf= +51,	cp=37
no,	dhf=+90,	dgf= +87	30
h2o	dhf=-242	dgf=-229	34
nh3	dhf=-46	dgf= -16	35
o2			29

We then find for combustion of NH_3 to NO :

$dhr = 90 + 1.5(-242) - (-46) = -227 \text{ kJ/mol}$
 $dgr = 87 + 1.5(-229) - (-16) = -240.5 \text{ kJ/mol}$
 $dcp = 30 + 1.5*34 - 35 - 1.25*29 = 9.75 \text{ (ved 298K)}$
 $dcp = 35 + 1.5*42 - 59 - 1.25*32 = -1 \text{ (ved 940C)}$
 $dcp \text{ mean ca. } 4 \text{ J/mole K}$

Heat of reaction at 940C: $-227 + 4e-3*915 = -223 \text{ kJ/mol}$