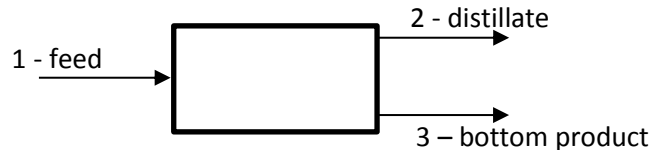


BALANCES

Balance of a distillation unit

10 kmol of a feed containing 55 mol. % of a component A and 45 mol. % of B was processed in a distillation unit. 5 kmol of distillate with composition of 90 mol. % of A was obtained. What are the amount and composition of the bottom product?

Solution: 1. Schematics of the distillation unit.



Matrix of the problem: a simple table in which columns contain data concerning each stream, the first row total number of moles for each stream and the rest composition expressed in molar fractions. The table will be 3 x 3 for this problem.

	1	2	3
n / kmol	10	5	n_3
A	0.55	0.9	$x_{A,3}$
B	0.45	0.1	$x_{B,3}$

We can easily see from the table that the number of unknowns is 3. To solve the problem, we need to write down three independent equations. These equations will be: 2 mass balances and the condition that the sum over molar fractions in each stream is equal to one.

$$10 = 5 + n_3$$

$$10 \cdot 0.55 = 0.9 \cdot 5 + x_{A,3} n_3$$

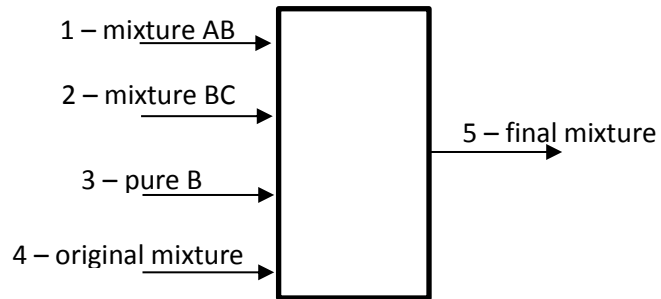
$$1 = x_{A,3} + x_{B,3}$$

This set of equations can easily be solved yielding the following results: $n_3 = 5$ kmol, $x_{A,3} = 0.2$, and $x_{B,3} = 0.8$.

Balance of the preparation of a mixture with a given composition

300 kg of a mixture containing 10 wt. % of a component A, 10 wt. % of B and 80wt % of C is in a storage tank. The goal is to obtain 500 kg of a mixture with the composition of 20 wt. % of A, and 30 wt. % of B. The following is available: a mixture AB containing 90 wt.% of A and 10 wt. % of B, A mixture of BC containing 8 wt. % of B and 92 wt. % of C, and pure component B. What amounts of mixtures AB and BC and pure component B have to be added to the original mixture?

Solution: Schematics of the problem.



Matrix of the problem:

	1	2	3	4	5
m /kg	m_1	m_2	m_3	300	500
w_A	0.9	0	0	0.1	0.2
w_B	0.1	0.08	1	0.1	0.3
w_C	0	0.92	0	0.8	0.5

The number of unknowns is three, i. e. we need three independent equations to solve this problem. The three independent equations are mass balances:

1. total balance: $m_1 + m_2 + m_3 + 300 = 500$
2. balance of comp. A: $0.9m_1 + 300 \cdot 0.1 = 500 \cdot 0.2$
3. balance of comp. C: $0.92m_2 + 300 \cdot 0.8 = 500 \cdot 0.5$

This set of equations can easily be solved yielding the following results: $m_1 = 77.78$ kg, $m_2 = 10.87$ kg, $m_3 = 111.35$ kg.

FLUID TRASPORT

Input power of a pump and energy consumption.

Water is pumped from an open well into a closed reservoir where a constant overpressure of 0.02 MPa is kept. The height difference in water levels in the well and the reservoir is 25 m, the cross-sections of the well and the reservoir are essentially identical. Water flows through a plastic pipe with a mean velocity of 1 ms^{-1} and its temperature is 10 DC ($\rho = 1000 \text{ kg m}^{-3}$, $\eta = 1.3 \times 10^{-3} \text{ Pa s}$). The tubing is 28 m long, its inner diameter is 32 mm, and contains fittings (saci kos, uzaviraci ventl, kolena 90 s.) Calculate the input power of a pump shaft, input power of the electromotor and a daily energy consumption if the total efficiency of pumping is 60 % and the efficiency of electromotor is 74 %.

Data: Density of water $\rho = 1000 \text{ kg m}^{-3}$; dynamic viscosity of water $\eta = 1.3 \times 10^{-3} \text{ Pa s}$; pressure in the well $p_1 = p_{\text{ATM}} = 101325 \text{ Pa}$; pressure in the reservoir $p_2 = p_{\text{ATM}} + 20000$; inner diameter of the pipe $d = 0.032 \text{ m}$; the length of the pipe $L = 28 \text{ m}$; mean velocity of the water: $v = 1.2 \text{ ms}^{-1}$; pumping height difference $h = 25 \text{ m}$; efficiency of the pump $\eta_c = 0.6$; efficiency of the electromotor $\eta_{\text{el}} = 0.74$.

Solution:

We will use Bernoulli equation with a term corresponding to the energy supplied by the pump. This equation reads: $\frac{p_1}{\rho} + \frac{v_1^2}{2} + gz_1 + e_c = \frac{p_2}{\rho} + \frac{v_2^2}{2} + gz_2 + e_{\text{dis}}$. One can rearrange the equation to arrive at the expression for the e_c . $e_c = \frac{p_2 - p_1}{\rho} + \frac{v_2^2 - v_1^2}{2} + g(z_2 - z_1) + e_{\text{dis}}$. In this equation, the second term on the right side equals zero ($v_1 = v_2 = v$), the third term on the right side equals to hg , and e_{dis} can be calculated from $e_{\text{dis}} = \left(\lambda \frac{L}{d} \frac{v^2}{2}\right) + \left(\sum \zeta_j\right) \frac{v^2}{2}$, where the first term corresponds to the energy loss in a plastic pipe and the second on all fittings.

- calculation of the second term in e_{dis} : the coefficient ζ equals to 6 for suction basket, 3 for closing ventl and 2×1.26 for the two 90° elbow-pipes which gives $\sum \zeta_j = 12.52$
- calculation of the first term of e_{dis} : coefficient lambda will be calculated from one of the criterial equation chosen according to the value of Re

$$Re = \frac{vd\rho}{\eta} = \frac{1.2 \times 0.032 \times 1000}{1.3 \times 10^{-3}} = 29538. \text{ This number corresponds to turbulent regime.}$$

$$\text{the relative roughness defined as } \varepsilon_r = \frac{\varepsilon_a}{d} = \frac{0.01 \times 10^{-3}}{0.032} = 3.1 \times 10^{-4}$$

$$\text{Coefficient lambda will be calculated from: } \lambda = \frac{0.25}{\left\{ \log \left[\left(\frac{6.81}{Re} \right)^{0.9} + \frac{\varepsilon_r}{29538} \right] \right\}^2} = \frac{0.25}{\left\{ \log \left[\left(\frac{6.81}{29538} \right)^{0.9} + \frac{3.1 \times 10^{-4}}{29538} \right] \right\}^2} = 0.024$$

and the total power output of the pump: $e_c = \frac{p_2 - p_1}{\rho} + \frac{v_2^2 - v_1^2}{2} + g(z_2 - z_1) + e_{dis} = \frac{20000}{1000} + 25 \times 9.81 + \left(0.024 \frac{28}{0.032} + 12.52\right) \frac{1.2^2}{2} = 289.4 \text{ J kg}^{-1}$.

c) power input at the pump shaft: $P_c = \frac{e_c \dot{m}_c}{\eta_c} = \frac{e_c v \pi d^2 \rho}{\eta_c} = \frac{289.4 \times 1.2 \times 3.14 \times 0.032^2 \times 1000}{4 \times 0.6} = 465 \text{ W}$

d) power input of the electromotor: $P_z = \frac{P_c}{\eta_{el}} = \frac{465}{0.74} = 628 \text{ W}$.

e) Energy consumption: $E_z = P_z \tau = 628 \times 10^{-3} \times 24 = 15 \text{ kWh}$

Results: The power input at the pump shaft is 465 W, power input of the electromotor is 628 W and the daily consumption of energy is 15 kWh.

FILTRATION

Mass balance of a leaf filter

Water suspension with the density of 1150 kg/m^3 containing 14.2 % (w/w) of solid particles is filtered at constant pressure in a leaf-and-shell filter. 1.83 m^3 of the filtrate is obtained in 5 minutes during a laboratory filtration. The filter cake contains 27.5% moisture (w/w). The filtration was carried out at 20 DC. What is performance of the filter (expressed as volume of the processed suspension in 24 hours), when the time of filtration is extended to 12 minutes, the washing of the filtration cake takes 15 minutes and preparation of filter for the next filtration round takes 25 minutes?

Data: density of suspension: $\rho_S = 1150 \text{ kgm}^{-3}$; mass fraction of solid particles in the suspension: $w_S = 0.142$, cake moisture: $w_{IC} = 0.275$; time of laboratory filtration: $\tau_{F1} = 300 \text{ s}$; volume of the filtrate in laboratory filtration: $V_{F1} = 1.85 \text{ m}^3$; extended time of filtration: $\tau_{F2} = 720 \text{ s}$; time of cake washing: $\tau_w = 900 \text{ s}$; time of idling : $\tau_i = 1500 \text{ s}$

Solution:

1. Duration of one filtration cycle: $\tau_t = \tau_{F2} + \tau_w + \tau_i = 720 + 900 + 1500 = 3120 \text{ s}$

2. Number of filtration cycles realizable in 24 hours: $C = \frac{24 \cdot 3600}{\tau_t} = 27.7$

3. Volume of the filtrate obtained in τ_{F2} : The volume of the filtrate is directly proportional to the time of filtration in case of filtration performed at constant filtration rate: $V_{F2} = \frac{\tau_{F2}}{\tau_{F1}} V_{F1} = \frac{720}{300} 1.85 = 4.44 \text{ m}^3$

4. The mass of the filtrate is $m_{F2} = V_{F2} \rho_F = 4.44 \cdot 998.19 = 4430 \text{ kg}$ (density of filtrate at 20 °C from tables)

5. The mass of suspension filtered in one filtration cycle from the total balance and the balance for the solid phase: $m_S = m_K + 4430$; $0.142 m_S = (1 - 0.275) m_K$

$$m_S = \frac{4430}{1 - \frac{0.142}{1150}} = 5509 \text{ kg}$$

6. The volume of the filtered suspension in one cycle: $V_S = \frac{m_S}{\rho_S} = \frac{5509}{1150} = 4.79 \text{ m}^3$

7. The performance of the filter: $V_{Sc} = CV_S = 27.7 \cdot 4.79 = 132.7 \doteq 133 \text{ m}^3$

Results: The performance of the filter is 133 m^3 of the suspension filtered in 24 hours.

Volume balance in a filter press

A filter press with 25 frames with dimensions of 500 x 500 x 35 mm is used for filtration of waste slurries from a metallurgical production plant. The slurry contains 7 vol % of solid particles and the moisture of the filter cake is 24 vol %. The filtration time is 4250 s. The filter cake is washed with water whose volume is 15 % of the total filtrate volume. Filtration and washing takes places at the same constant filtration rate. What is the performance of the filter press in 24 hours when cake removal and press filter re-assembly takes 50 minutes?

Data: number of press filter frames: $n=24$; dimensions of the frames: $a \times b \times c = 0.5 \times 0.5 \times 0.035$ m; volume fraction of solid particles in the suspension: $\varphi_S = 0.07$; volume fraction of the moisture in the cake: $\varphi_{l,K} = 0.24$; time of filtration: $\tau_F = 4250$ s; volume of the washing medium: $V_w = 0.15 V_F$; time of idling: $\tau_i = 3000$ s

Solution: To determine the performance of the filter we need to calculate the duration of one filtration cycle that requires the knowledge of the time of cake washing (the filtration time and the idling time are known).

1. We will assume that the cake fills up the frames of the filter press and thus its volume can be calculated as: $V_K = nabc = 25 \cdot 0.5 \cdot 0.5 \cdot 0.035 = 0.219m^3$.

2. Calculation of the suspension volume processed in one cycle and the volume of the filtrate from the volume balances: $V_S = V_F + 0.219$; $0.07V_S = (1 - 0.24)0.219$

$$V_S = \frac{(1 - 0.24)0.219}{0.07} = 2.375m^3$$

$$V_F = V_S - 0.219 = 2.375 - 0.219 = 2.156m^3$$

3. Volume of the washing water is: $V_w = 0.15V_F = 0.15 \cdot 2.156 = 0.3234m^3$

4. Time of washing is given by (considering same constant filtration and washing rates):

$$\tau_w = \frac{V_w}{V_F} \tau_F = \frac{0.3234}{2.156} 4250 = 637.5 \text{ s}$$

5. Total time of one filtration cycle: $\tau_t = \tau_F + \tau_w + \tau_i = 4250 + 637.5 + 3000 \doteq 7900$ s

6. Number of filtration cycles in 24 hours: $C = \frac{24 \cdot 3600}{\tau_t} = 10.94$

7. The performance of the filter: $V_{Sc} = CV_S = 10.94 \cdot 2.375 = 26 m^3$

Results: The performance of the filter is $26 m^3$ of the suspension filtered in 24 hours.

Filtration at constant filtration rate in a nutch filter

100 kg/hour of a mother liquor containing solid crystals is required to be filtered in a nutch filter with filtration area of 3.25 m^2 . The mother liquor possesses density of 1098 kg/m^3 and contains 15 wt. % of crystals. Filtration cake contains 88 wt.% of crystals and 12 wt.% of the mother liquor. Filtration runs at constant velocity, the crystals in the cake are not washed and the time needed for assembling the nutch is 20 minutes. Determine, whether the filtration in a given nutch can be used to proces 100 kg/hour of the mother liquor. The values of filtration constants are: $K_F = 3.2 \times 10^{-7} \text{ m}^2\text{s}^{-1}$ (value at the end of filtration) and $q_m = 4.5 \times 10^{-3} \text{ m}$.

Data: filtration cross-sectional area: $S_F = 3.25 \text{ m}^2$; duration of one filtration cycle: $\tau_t \leq 1 \text{ h}$; time of idling: $\tau_i = 1200 \text{ s}$; $\tau_w = 0$ (no washing of the cake); mass of suspension in one cycle: $m_S = 100 \text{ kg}$; mass fraction of solid particles in the suspension: $w_S = 0.15$; mass fraction of solid particles in the cake: $w_K = 0.88$; filtrate density: $\rho_F = 1098 \text{ kgm}^{-3}$; filtration constants: $K_F = 3.2 \times 10^{-7} \text{ m}^2\text{s}^{-1}$ and $q_M = 4.5 \times 10^{-3} \text{ m}$.

Solution:

1. The mass of the cake from mass balance: $m_K = \frac{w_S m_S}{w_K} = \frac{0.15 \cdot 100}{0.88} = 17.05 \text{ kg}$

2. The mass of filtrate produced in one filtration cycle: $m_F = m_S - m_K = 100 - 17.05 = 82.95 \text{ kg}$

3. Volume of the filtrate: $V_F = \frac{m_F}{\rho_F} = \frac{82.95}{1098} = 7.555 \times 10^{-2} \text{ m}^3$

4. Volume of the filtrate per filtration cross-sectional area: $q_F = \frac{V_F}{S_F} = \frac{7.555 \times 10^{-2}}{3.25} = 2.325 \times 10^{-2} \text{ m}$

5. Time of filtration at constant filtration rate: $\tau_F = \frac{q_F(q_F + q_M)}{K_F} = \frac{2.325 \times 10^{-2}(2.325 \times 10^{-2} + 4.5 \times 10^{-3})}{3.2 \times 10^{-7}} = 2016 \text{ s}$

6. Duration of one filtration cycle: $\tau_t = \tau_F + \tau_w + \tau_i = 2016 + 1200 + 0 = 3216 \text{ s}$

Results: The filtration can be realized since the duration of one filtration cycle (3216 s) is shorter than one hour.

Filtration at constant filtration pressure difference, determination of filtration constants

Cell suspension of bacterium *Bacillus subtilis* is filtered at constant filtration pressure difference with the goal to separate cells from liquid cell growth medium. One determined the following values by using a laboratory filter with filtration area of 0.25 m^2 and filtration pressure difference of 48 kPa: 12.1 dm^3 was obtained in 3 min and 32 dm^3 in 20 min. What should the area of a production filter be if we wanted to process 4 m^3 of the cell suspension at the filtration pressure difference of 75 kPa? The cell suspension contains 12 kg of cell mass in 1 m^3 . Filtration cake contains 23 wt. % of cell mass. Laboratory and the production filtration run at the same temperature and with the same filter medium used.

Data: filtration cross-sectional area of the laboratory filter: $S_{F,lab} = 0.25 \text{ m}^2$; pressure difference in filtration in a laboratory filter $\Delta p_{F,lab} = 48 \text{ kPa}$; times of filtration and corresponding filtrate volumes: $\tau_{F1} = 180 \text{ s}$; $V_{F1} = 1.21 \times 10^{-2} \text{ m}^3$, $\tau_{F2} = 1200 \text{ s}$; $V_{F2} = 3.2 \times 10^{-2} \text{ m}^3$; pressure difference in filtration in a industrial filter $\Delta p_F = 75 \text{ kPa}$; filtrate volumes obtained in the industrial filter: $V_F = 4 \text{ m}^3$; mass fraction of the cell mass in the suspension: $w_S = 12/1000 = 0.012$ (assuming the density of the cell suspension does not differ significantly from the density of water, which is taken to be equal to 100 kg/m^3 – this assumption is based on the fact that the concentration of cells in the suspension is very low); mass fraction of cell mass in the cake: $w_K = 0.23$;

Solution:

1. Calculation of $K_{f,lab}$ and q_M from the data obtained for laboratory filtration:

$$q_{F1} = \frac{V_{F1}}{S_{F,lab}} = \frac{1.21 \times 10^{-2}}{0.25} = 0.0484 \text{ m}; \quad q_{F2} = \frac{V_{F2}}{S_{F,lab}} = \frac{3.2 \times 10^{-2}}{0.25} = 0.128 \text{ m}$$

By substituting these values into the corresponding filtration rate equation we get:

$$0.0484^2 + 2 \times 0.0484 q_M - 2 \times 180 K_{F,lab} = 0; \quad 0.128^2 + 2 \times 0.128 q_M - 2 \times 1200 K_{F,lab} = 0$$

The laboratory filtration constants are: $K_{F,lab} = 7.037 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ and $q_M = 1.97 \times 10^{-3} \text{ m}$.

2. Industrial filtration is operated at a different pressure difference and thus filtration constant for the industrial filter will be different from that one for the laboratory filter. Q_M is constant.

$$K_F = \frac{\Delta p_F}{\Delta p_{F,lab}} K_{F,lab} = \frac{75}{48} 7.037 \times 10^{-6} \doteq 1.10 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$$

3. Calculation of q_F for the industrial filter

$$q_F^2 + 2 \times q_F 1.97 \times 10^{-3} - 2 \times 1800 \times 1.1 \times 10^{-5} = 0$$

4. Calculation of filtrate volume from mass balances and assumption of water density equal to 1000 kg/m^3 :

$$4000 = m_F + m_K; \quad 0.012 \times 4000 = 0.23 m_K$$

EXTRACTION WITH IMMISCIBLE SOLVENTS

The consumption of the solvent in repeated extraction

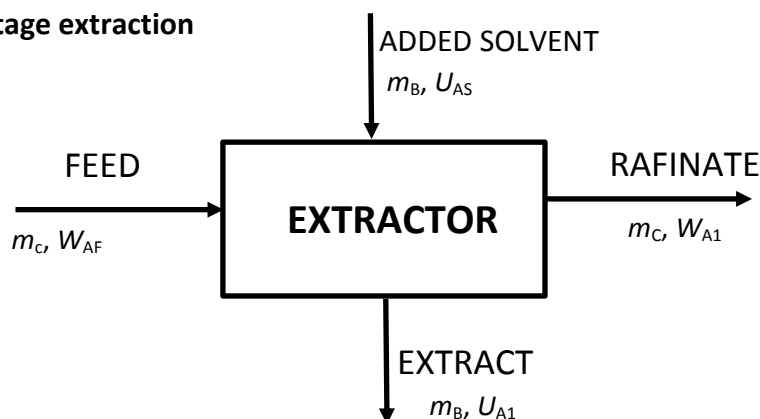
A mixture with the composition of 6.8 wt% of acetone and 93.2 wt. % of water is extracted with pure o-xylene. 65% of the acetone is to transfer into the extract. Determine the required amount of extracting solvent for one kilogram of the feed in case of one stage equilibrium extraction and repeated extraction in two stages. Calculate the final concentration of acetone in combined extracts for the repeated extraction if we use the same amount of solvent in both stages. Extraction runs at 30 °C.

Data: A – acetone (extracted component), B – o-xylene (added solvent), C – water (original solvent). Equilibrium for this system can be found on: <http://uchi.vscht.cz/index.php/en/studium/uplatneni-absolventu/e-tabulky> (data copied in the table below). The solvents are mutually immiscible (this statement is based on the equilibrium data), $w_{AF} = 0.068$; $u_{AS} = 0$; $\theta = 0.65$ (65 % of acetone transfers into extract). This is also the reason why we will use relative mass fractions for solving this problem.

Equilibrium:

Mass fraction of acetone		Relative mass fraction of acetone	
Water phase	Xylene phase	Water phase	Xylene phase
0.0091	0.0060	0.0092	0.0060
0.0180	0.0119	0.0183	0.0120
0.0357	0.0231	0.0370	0.0236
0.0519	0.0368	0.0547	0.0382
0.0796	0.0619	0.0865	0.0660
0.0900	0.0685	0.0989	0.0735
0.1590	0.1367	0.1891	0.1583
0.2200	0.2005	0.2821	0.2508

SOLUTION: One stage extraction



Schematics of the process: one-stage extraction, the output streams raffinate and extract are in equilibrium.

1. Calculation of W_{AF} : $W_{AF} = \frac{w_{AF}}{1-w_{AF}} = \frac{0.068}{1-0.068} = 0.073$

2. $U_{AS} = 0$ (no acetone in the added solvent)

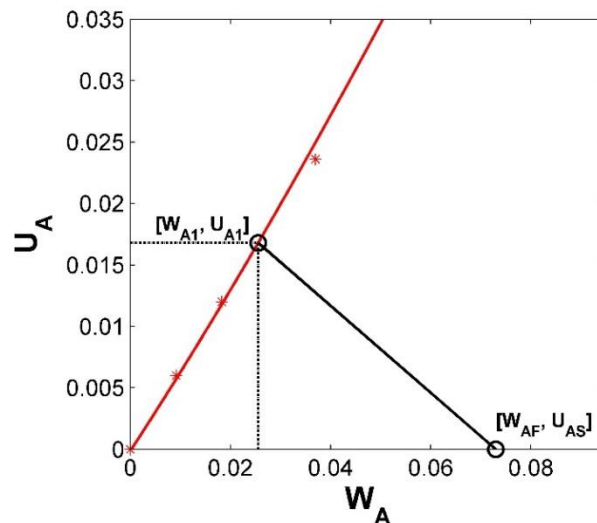
3. Calculation of the acetone concentration in the raffinate:

$$m_{A1} = (1 - \theta)m_{AF}$$

$$m_C W_{AF} = (1 - \theta)m_C W_{AF}$$

$$W_{A1} = (1 - \theta)W_{AF} = (1 - 0.65) \cdot 0.073 = 0.0256$$

4. Using the assumption that the output streams from the extractor are in equilibrium allows us to determine the concentration of the acetone in extract. Here, we will use a graphical method. Figure below shows a red line that represents the equilibrium line for the system acetone – water - o-xylene. Relative mass fraction of acetone in water (original solvent) is plotted on the x axis, relative mass fraction of acetone in o-xylene on the y axis. The equilibrium points are from the table above, the solid red line is a polynomial fit (3rd order). The graph is zoomed in on the range that is convenient for our calculation. We will draw a line perpendicular to the x axis that crosses the x coordinate in W_{A1} . The intersection of this line with the equilibrium line yields the concentration of the acetone in the extract U_{A1} . The value of the concentration is read off from the y axis: $U_{A1} = 0.0165$. The solid line connecting points $[W_{AF}, U_{AS}]$ and $[W_{A1}, U_{A1}]$ is the operational line.



5. To calculate the amount of the added solvent needed for processing of 1 kg of the feed we will start with the mass balance of the acetone. This equation reads:

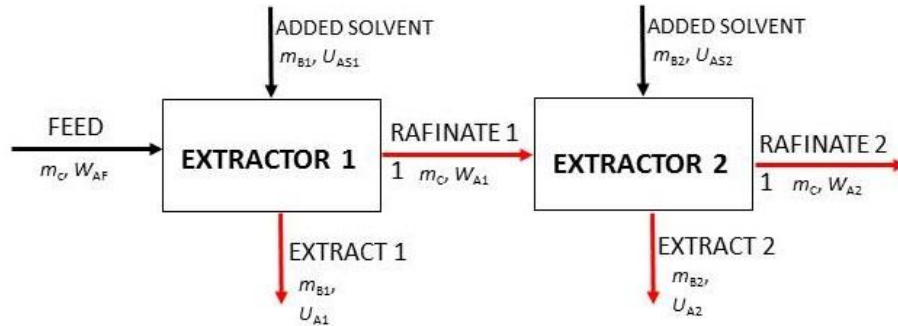
$$m_C W_{AF} + m_B U_{AS} = m_C W_{A1} + m_B U_{A1} \text{ where } m_C \text{ can be calculated from:}$$

$$m_C = m_F(1 - w_{AF}) = 1 \cdot (1 - 0.068) = 0.932 \text{ kg}$$

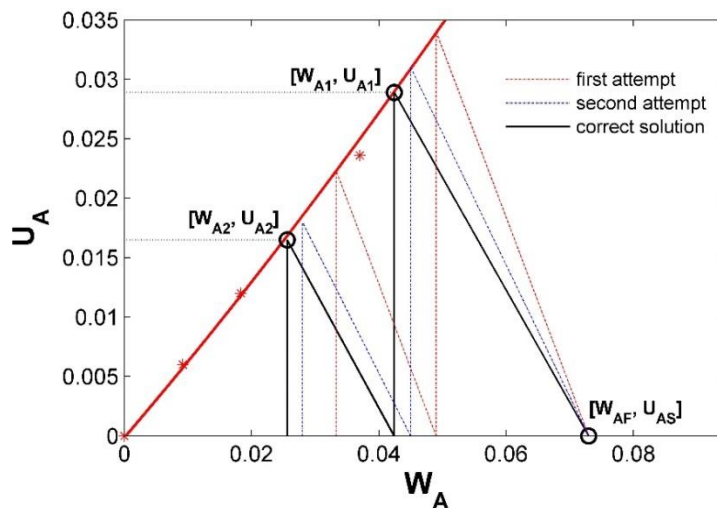
6. The component balance above can be rearranged into a form that allows to calculate the amount of added solvent. Since this solvent is pure ($u_{AS}=0$), this is also the amount of solvent required for processing of 1 kg of the feed.

$$m_B = m_C \frac{(W_{AF} - W_{A1})}{U_{A1}} = 0.932 \frac{(0.073 - 0.0256)}{0.0165} = 2.68 \text{ kg}$$

SOLUTION: Two-stage extraction



Schematics of a two-stage extraction: Streams leaving the first and second stage are in equilibrium (red arrows). Because we are to use the same amount of added solvent in both stages, m_{B1} equals m_{B2} . The concentrations of acetone in raffinate and extract leaving the second stage are equal to W_{A1} and U_{A1} from the single stage extraction. The goal is thus to calculate the output concentrations from the first stage of the two-stage extraction under the condition that m_{B1} equals m_{B2} . Using a graphical solution (see figure below), we are to draw two operational lines that are parallel (the slope of the operational lines $-m_C/m_B$ is constant) where the first one starts in $[W_{AF}, U_{AS}]$ and the second one ends in $[W_{A2}, U_{A2}]$ having coordinates of $[0.0256, 0.0165]$. These two operational lines are drawn by trial-and-error method. We will draw the first line connecting $[W_{AF}, U_{AS}]$ with a point $[W_{A1,1}, U_{A1,1}]$ lying on the equilibrium line. The second operational line having the same slope as the first one will start in point $[W_{A1,1}, U_{AS}]$ and will cross equilibrium in a point $[W_{A2,1}, U_{A2,1}]$. If this point has coordinates of $[0.0256, 0.0165]$, we are done, if not we have to adjust the slope of the equilibrium lines so that we get closer to the required output concentrations from the second stage. This process is repeated until we arrive at the correct point.

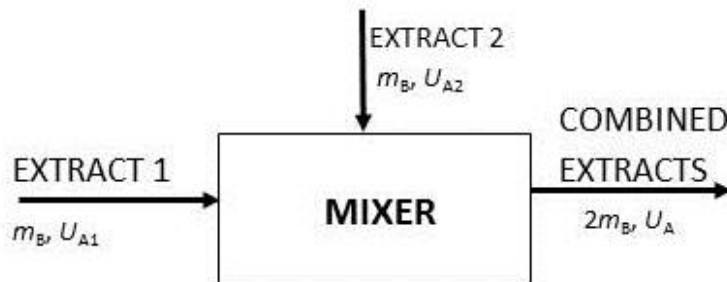


The coordinates of $[W_{A1}, U_{A1}]$ read off from the graph are $[0.0424, 0.0289]$. Known values of this point can now be used for calculating the required amount of added solvent used in both stages. Starting from a mass balance for acetone either in the first stage and rearrangement we can arrive at expression:

$$m_B = m_C \frac{(W_{AF} - W_{A1})}{U_{A1}} = 0.932 \frac{(0.073 - 0.0424)}{0.0289} = 0.987 \text{ kg.}$$

The total consumption of solvent is 1.97 kg.

The final concentration of acetone in combined extracts from the first and second stage will be calculated from a total balance of a mixer with two input streams and output stream:



The balance then reads:

$$m_B U_{A1} + m_B U_{A2} = 2m_B U_A$$

$$U_A = \frac{U_{A1} + U_{A2}}{2} = \frac{0.0289 + 0.0165}{2} = 0.0227$$

The relative mass fraction should be converted to mass fraction:

$$u_A = \frac{U_A}{1 + U_A} = \frac{0.0227}{1 + 0.0227} = 0.0222.$$

CONCLUSIONS: The consumption of the solvent in one- and two-stage extractions are 2.68 and 1.97 kg. The concentration of acetone in combined extracts is 2.22 wt.%.

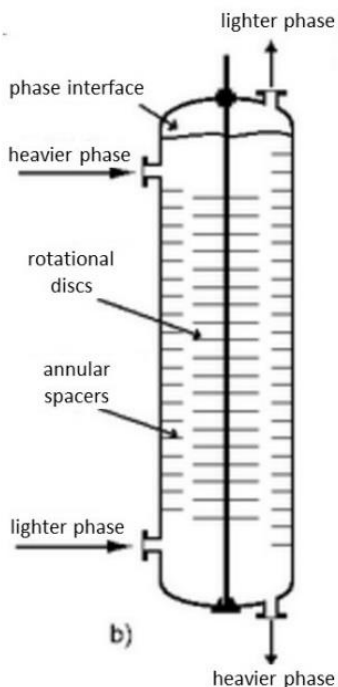
Calculation of HETP (height equivalent to theoretical plate)

Determine HETP of a counter-current rotational disc column 2.7 m high. Water phase containing 7 wt. % of acetone and o-xylene phase containing 0.5 wt. % of acetone enter the column. The content of acetone in the output water and o-xylene phases is 1.95 and 3.85 wt. %, respectively. What is the ratio of mass flow rates of the entering phases? What is the maximum possible concentration of acetone in the leaving extract? The extractor is operated at 30 °C.

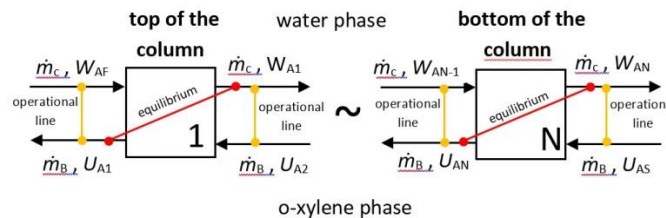
DATA: A: extracted component, B: added solvent, C: original solvent, mass fraction of acetone in the feed $w_{AF} = 0.07$; mass fraction of acetone in the solvent $u_{AS} = 0.005$; mass fraction of acetone in the raffinate $w_{AN} = 0.0195$; mass fraction of acetone in the extract $u_{A1} = 0.0385$; the height of the column $h = 2.7$ m. Equilibrium for this system can be found on: <http://uchi.vscht.cz/index.php/en/studium/uplatneni-absolventu/e-tabulky> (data copied in the table below). The equilibrium data suggests the immiscibility of the solvents which automatically leads to the use of relative mass fractions.

Equilibrium:

Mass fraction of acetone		Relative mass fraction of acetone	
Water phase	Xylene phase	Water phase	Xylene phase
0.0091	0.0060	0.0092	0.0060
0.0180	0.0119	0.0183	0.0120
0.0357	0.0231	0.0370	0.0236
0.0519	0.0368	0.0547	0.0382
0.0796	0.0619	0.0865	0.0660
0.0900	0.0685	0.0989	0.0735
0.1590	0.1367	0.1891	0.1583
0.2200	0.2005	0.2821	0.2508



SCHEMATICS of the problem: A schematic of a real counter-current extraction column with rotational discs on the left, a schematic of the problem used in calculation on the right.



the right.

The density of o-xylene is lower than that of water. Therefore, o-xylene is the lighter phase and water is the heavier phase.

Solution:

We will use graphical method to solve the problem. In the first step, we will draw equilibrium curve using the data from the table above. Because the solvents are immiscible (inferred from the equilibrium data) we will use relative mass fractions in calculations. In the figure below, the equilibrium is represented with a red curve that connects the equilibrium data from the table. To recall, the streams leaving a theoretical plate are in equilibrium, i. e. the composition of these streams is also equilibrium composition (red line in the schematic above). In the next step we will draw operational line. This operational line corresponds to the mass balance of the extractor. The compositions of streams that are on the same side of a stage has to lie on this line (orange line in the schematic above). The knowledge of compositions of all streams leaving or entering the extractor allows us to draw to operational line in the graph. This operational line connects points $[W_{AF}, U_{A1}]$ and $[W_{AN}, U_{AS}]$.

$$W_{AF} = \frac{w_{AF}}{1 - w_{AF}} = \frac{0.07}{1 - 0.07} = 0.073$$

$$W_{AN} = \frac{w_{AN}}{1 - w_{AN}} = \frac{0.0195}{1 - 0.0195} = 0.02$$

$$U_{AS} = \frac{u_{AS}}{1 - u_{AS}} = \frac{0.005}{1 - 0.005} = 0.005$$

$$U_{A1} = \frac{u_{A1}}{1 - u_{A1}} = \frac{0.0385}{1 - 0.0385} = 0.04$$

To obtain the number of theoretical plates we will solve the problem by finding the compositions of all streams that enter or leave each of the theoretical plates. We will start on the left of the column (stage 1) where the composition of the feed and extract are given by a point $[W_{AF}, U_{A1}]$. We will find the composition of the water phase leaving the stage one by plotting a line parallel to x axis starting in point $[W_{AF}, U_{A1}]$ and ending in the corresponding point lying on the equilibrium line. This point has coordinates $[W_{A1}, U_{A1}]$. Now using the operational line, we will find the composition of the o-xylene phase entering stage 1. We will simply plot a line parallel to y axis that starts in point $[W_{A1}, U_{A1}]$ and ends in the corresponding point lying on the operational line. This point has coordinates $[W_{A1}, U_{A2}]$. We repeat this process until we get into or beyond the point $[W_{AN}, U_{AS}]$. We see that we obtained three full "stairs" corresponding to three full theoretical plates and part of the fourth one. To quantify how much of the fourth step we obtained we simply evaluate the ratio of $\frac{LM}{KM} = \frac{W_3 - W_{AN}}{W_3 - W_4} = 0.65$. The extraction column, thus, has 3.65 theoretical plates. To evaluate HETP, we divide the height of the column with the number of theoretical plates: $HETP = \frac{h}{N_T} = \frac{2.7}{3.65} = 0.74 \text{ m}$.

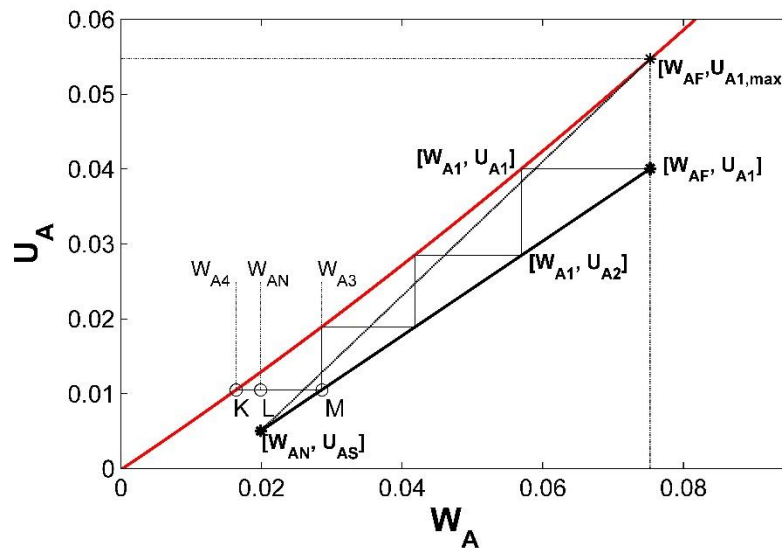
The ratio of the mass flow rates of the entering phases (i. e. mass flow rate of the feed and the mass flow rate of the added solvent) will be calculated from: $\frac{\dot{m}_F}{\dot{m}_S} = \frac{\dot{m}_{AF} + \dot{m}_C}{\dot{m}_{AS} + \dot{m}_B} = \frac{W_{AF}\dot{m}_C + \dot{m}_C}{U_{AS}\dot{m}_B + \dot{m}_B} = \frac{\dot{m}_C(1+W_{AF})}{\dot{m}_B(1+U_{AS})}$ where the ratio $\frac{\dot{m}_C}{\dot{m}_B}$ will be evaluated from the component balance of A for the whole extractor: $\frac{\dot{m}_C}{\dot{m}_B} = \frac{(U_{A1} - U_{AS})}{(W_{AF} - W_{AN})} = \frac{(0.04 - 0.005)}{(0.075 - 0.02)} = 0.63$. The required ratio of mass flow rates is: $\frac{\dot{m}_F}{\dot{m}_S} = 0.63 \frac{(1+0.075)}{(1+0.005)} = 0.67$.

We obtain maximum concentration of acetone in the extract when \dot{m}_B corresponds to the minimum consumption of the solvent $\dot{m}_{B,min}$. In the graphical solution, the operational line with $\dot{m}_{B,min}$ (it is the

operational line crossing point $[W_{AN}, U_{AS}]$ with maximal possible slope) is plotted with dashed black line.

We will read off $U_{A1,max} = 0.0545$. The mass fraction is then:

$$u = \frac{U_{A1}}{1-U_{A1}} = \frac{0.0545}{1-0.0545} = 0.052.$$



Graphical solution of the given problem.

Conclusions: The HETP of the column is 0.74 m, the ratio of mass flow rates of entering phases is The HETP of the column is 0.74 m, the ratio of mass flow rates of entering phases is 0.67 and the maximum possible concentration of acetone in extract is 5.2 wt. %.

DISTILLATION

Calculation of liquid – vapor equilibrium

Compare calculated boiling and dew points of a mixture of aniline and benzene containing 30 mol.% of benzene with experimental data (at normal pressure). Calculate the relative volatility α_{AB} for the mixture of benzene and aniline from the tabulated experimental data and compare with relative volatility calculated from saturated vapor pressures of pure components $\alpha_{AB} = p_A^\circ / p_B^\circ$.

Solution:

Benzene will be component A and aniline component B. We know the total pressure $p = 101325$ Pa and the molar fraction of benzene in the liquid $x_A = 0.3$ for determining the boiling point T_b and in the vapor $y_A = 0.3$ for determining the dew point T_d . We will find the experimental data in a table available on departmental website ([place the reference](#)). These data are for equilibrium composition of a mixture of benzene – aniline at normal pressure:

$$x_A = 0.3 \text{ ----> } y_A = 0.94; T_b = 108.4^\circ\text{C}$$

$$y_A = 0.3 \text{ ----> } x_A = 0.0237; T_d = 172.1^\circ\text{C (using interpolation).}$$

Next, we will use Antoine equation to calculate the saturated vapor pressures. The coefficients for Antoine equation for both components can also be found in a table on departmental website:

$$p_A^\circ(T) = \exp\left(13.82649 - \frac{2755.641}{(T - 53.989)}\right)$$

$$p_B^\circ(T) = \exp\left(15.17245 - \frac{4238.575}{(T - 56.277)}\right)$$

where the temperature is in Kelvins and the saturated vapor pressures of components in kPa.

1. We will calculate the boiling point of the mixture for $x_A = 0.3$ from equation:

$$101.325 = 0.3p_A^\circ(T_b) + 0.7p_B^\circ(T_b)$$

After solving the equation, we obtain the boiling point $T_b = 394\text{K} = 120.9^\circ\text{C}$. The corresponding equilibrium composition of the vapor phase at this temperature is according to the Raoult law

$$\text{equal to: } y_A = x_A \frac{p_A^\circ(T_b)}{p} = 0.3 \frac{p_A^\circ(394)}{103.325} = 0.9045$$

2. The dew point of the mixture will be found in a similar way for $y_A = 0.3$ from equation:

$$1 = 0.3 \frac{101.325}{p_A^\circ(T_d)} + 0.7 \frac{101.325}{p_B^\circ(T_d)}$$

The dew point is: $T_d = 445.9\text{K} = 172.8^\circ\text{C}$. The equilibrium composition of the liquid phase at this

$$\text{temperature is according to Raoult law: } x_A = y_A \frac{p}{p_A^\circ(T_d)} = 0.3 \frac{101.325}{p_A^\circ(445.9)} = 0.0340$$

3. The relative volatility at 108.4°C calculated from the experimental data is equal to:

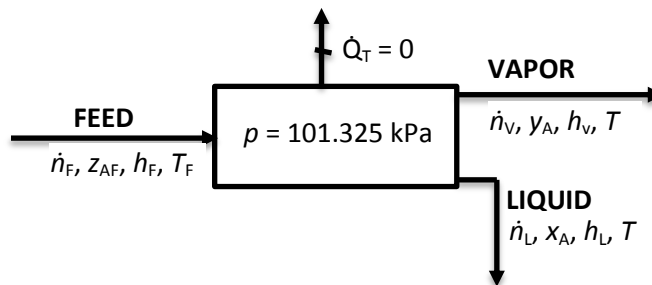
$$\alpha_{AB} = \frac{y_A/x_A}{y_B/x_B} = \frac{0.94/0.3}{0.06/0.7} = 36.6.$$

Relative volatility calculated from the saturated vapor pressures of components is: $\alpha_{AB} = \frac{p_A^{\circ}(381.55)}{p_B^{\circ}(381.55)} = \frac{224.21}{8.51} = 26.3.$

Calculation of flash distillation

Flash distillation is used to obtain liquid phase containing 80 mol.% of toluene from a mixture with composition of 50 mol.% of acetone and 50 mol.% of toluene. The process is adiabatic under the pressure of 101325 Pa. Find the temperature of the flash distillation and the composition of the distillate. Calculate the required temperature of the feed and the relative amount of obtained vapor and liquid phase.

Schematics:



Solution:

Component A: acetone, component B: toluene; the composition of the streams: $z_{AF} = 0.5$; $x_B = 0.8$ and the pressure in the drum is $p = 101325$ Pa. We will choose $\dot{n}_F = 1$ mol/s. The composition of the vapor phase can be obtained from equilibrium for given composition of the liquid phase $x_A = 1 - x_B = 0.2$ and pressure of 101325 Pa. The composition of the vapor phase is $y_A = 0.6553$ and the temperature of the distillation is $T = 82.86^\circ\text{C}$.

We will use molar balances to calculate molar flow rates of the vapor and liquid phases:

$$1 = \dot{n}_V + \dot{n}_L$$

$$1 \cdot 0.5 = 0.2\dot{n}_L + 0.6553\dot{n}_V$$

By solving this set of two equations with two unknowns we get: $\dot{n}_L = 0.528$ mol/s and $\dot{n}_V = 0.472$ mol/s.

The required temperature of the feed will be calculated from enthalpy balance. The mean molar heat capacities and enthalpies are:

$$\langle c_{pA}^{(l)}(41^\circ\text{C}) \rangle = 2.25 \text{ kJ/kg/K} = 130.6 \text{ J/mol/K}, \Delta h_{\text{vap},A}(82.8^\circ\text{C}) = 29.7 \text{ kJ/mol}$$

$$\langle c_{pB}^{(l)}(41^\circ\text{C}) \rangle = 1.75 \text{ kJ/kg/K} = 161 \text{ J/mol/K}, \Delta h_{\text{vap},B}(82.8^\circ\text{C}) = 34.8 \text{ kJ/mol}$$

The molar enthalpies of the feed, liquid and vapor with respect to the reference temperature of $T_{\text{REF}} = 0^\circ\text{C}$ and reference liquid state are:

$$h_F = z_{\text{AF}} \langle c_{pA}^{(l)} \rangle (T_F - T_{\text{REF}}) + z_{\text{BF}} \langle c_{pB}^{(l)} \rangle (T_F - T_{\text{REF}}) = 0.5 \cdot 130.6 \cdot (T_F - 0) + 0.5 \cdot 161 \cdot (T_F - 0) = 145.8 \cdot (T_F - 0)$$

$$h_L = x_A \langle c_{pA}^{(l)} \rangle (T - T_{\text{REF}}) + x_B \langle c_{pB}^{(l)} \rangle (T - T_{\text{REF}}) = 0.2 \cdot 130.6 \cdot (82.86 - 0) + 0.8 \cdot 161 \cdot (82.86 - 0) = 12837 \text{ J/mol}$$

$$h_V = y_A \langle c_{pA}^{(l)} \rangle (T - T_{\text{REF}}) + x_B \langle c_{pB}^{(l)} \rangle (T - T_{\text{REF}}) + y_A \Delta h_{\text{vap,A}} + y_B \Delta h_{\text{vap,B}} = 0.6553 \cdot 130.6 \cdot (82.86 - 0) + (1 - 0.6553) \cdot 161 \cdot (82.86 - 0) + 0.6553 \cdot 29700 + (1 - 0.6553) \cdot 34800 = 43148 \text{ J/mol}$$

By substituting into the enthalpy balance we arrive at:

$$1 \cdot 145.8 \cdot (T_F - 0) = 0.472 \cdot 12837 + 0.528 \cdot 43148$$

and calculate the temperature of the feed: $T_F = 197.8^\circ\text{C}$.

If the tabulated equilibrium data were not available, we could use Raoult law to estimate the composition of the vapor phase: $1 = x_A \frac{p_A^\circ(T)}{p} + x_B \frac{p_B^\circ(T)}{p}$, where the saturated vapor pressures for A and B are: $p_A^\circ(T) = \exp\left(14.37283 - \frac{2787.488}{(T-43.486)}\right)$; $p_B^\circ(T) = \exp\left(13.98998 - \frac{3090.782}{(T-53.963)}\right)$.

By solving the equation above we arrive at $T = 363.46 \text{ K} = 90.31^\circ\text{C}$ and $y_A = 0.5674$.

Batch distillation with unknown composition of the liquid phase

Batch distillation at normal pressure is used to process 100 kg of a mixture with composition of 18 wt.% of ethanol and 82 wt.% of water. How many kilograms of distillate with mean composition of 48 wt.% of ethanol will be obtained and how much ethanol will transfer into the distillate? At what temperature do we have to stop the distillation? Assume, that the output vapor is in equilibrium with the liquid phase.

Solution:

A: ethanol, B: water; Because we will not use Raoult law or any relations derived from it we can solve the problem in mass balances: $m_F = 100$ kg (initial weight of the batch); $w_{AF} = 0.18$ (initial mass fraction of A in the batch); $w_{AD} = 0.48$ (required mean mass fraction of ethanol in the distillate)

The mass balances are:

$$m_F = m_D + m_W$$

$$m_F w_{AF} = m_D \bar{w}_{AD} + m_W w_{AW}$$

The differential mass balance is:

$$\ln \frac{m_F}{m_W} = \int_{w_{AW}}^{w_{AF}} \frac{dw_A}{u_A - w_A}$$

where u_A is the mass fraction of ethanol in vapor which is in equilibrium with w_A . By substituting into the equations above, we get:

$$100 = m_D + m_W$$

$$100 \cdot 0.18 = m_D \bar{w}_{AD} + m_W w_{AW}$$

$$\ln \frac{100}{m_W} = \int_{w_{AW}}^{w_{AF}=0.18} \frac{dw_A}{u_A - w_A}$$

We will calculate the solution for the set of equations above for a few chosen values of w_{AW} . The equilibrium data for the system water – ethanol are available on the departmental website. Chosen values w_A and u_A will be written into a table below. To calculate the integral in the third equation, we will use a trapezoid method. We will integrate in the intervals given by the equilibrium data. The integrated function $1/(u_A - w_A)$ and the course of integration will be written into the table.

w_A	u_A	$t/^\circ\text{C}$	$1/(u_A - w_A)$	S_k	sum(S_k)	m_w	m_D	w_{AD}
0.18	0.5916	86.21	2.430		0	100	0	0.5916
0.15	0.5641	87.21	2.415	$S_1 = 0.07268$	0.07268	92.99	7.01	0.5780
0.1	0.4911	89.60	2.557	$S_2 = 0.12430$	0.19698	82.12	17.88	0.5474
0.05	0.3541	93.36	3.288	$S_3 = 0.14612$	0.34310	70.96	29.04	0.4977
0.03	0.2581	95.53	4.384	$S_4 = 0.07672$	0.41982	65.72	34.28	0.4676
0.01	0.1094	98.31	10.06	$S_5 = 0.14444$	0.56426	56.88	43.12	0.4043

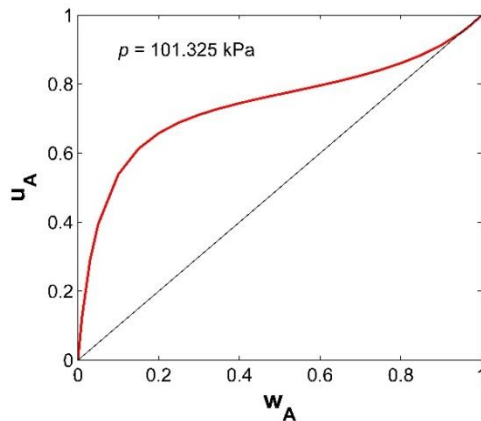
The column S_k is an approximation of the integral with **trapezoid rule**, e. g. the integral S_3 is:

$$S_3 = \int_{0.05}^{0.1} \frac{dw_A}{u_A - w_A} \doteq (0.1 - 0.05) \frac{(2.557 + 3.288)}{2} = 0.14612$$

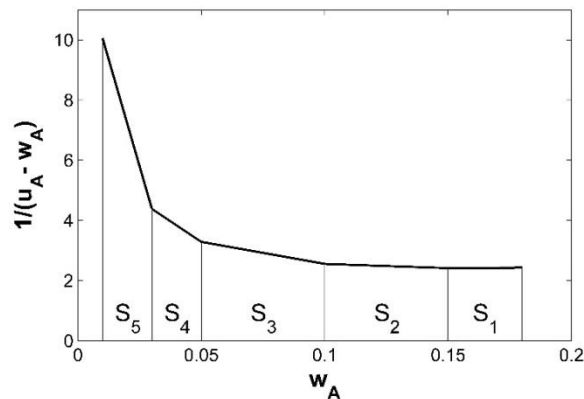
The column sum(S_k) is the sum of areas of several trapezoids, e. g. on a row for $w_{AW} = 0.05$ we have:

$$\sum S_k = \int_{0.05}^{0.18} \frac{dw_A}{u_A - w_A} = S_1 + S_2 + S_3 = \int_{0.15}^{0.18} \frac{dw_A}{u_A - w_A} + \int_{0.10}^{0.15} \frac{dw_A}{u_A - w_A} + \int_{0.05}^{0.10} \frac{dw_A}{u_A - w_A}$$

We will estimate the solution $w_{AW} = 0.0382$ from the table since at this composition of the liquid phase the mean mass fraction of A in the distillate is $w_{AD} = 0.48$. We will obtain $m_D = 32.10$ kg of the distillate. The batch distillation will be terminated at the temperature of $t = 94.64^\circ\text{C}$. The fraction of ethanol that has transferred into the distillate is: $\frac{m_D \bar{w}_{AD}}{m_F w_{AF}} \cdot 100\% = \frac{32.10 \cdot 0.48}{100 \cdot 0.18} \cdot 100\% = 85.6\%$.



The equilibrium liquid-vapor for the system ethanol – water.



The integration of $1/(u_A - w_A)$ using the trapezoid rule.

DRYING

Calculation of drying in a tray dryer

A sample containing 2.5 kg of a dry material and 0.67 kg of water was inserted in a tray dryer. The critical and the equilibrium moisture contents of the material obtained from experimental data were $W_{Ac} = 0.14$ and $W_A^* = 0.05$. The mass of the sample decreased by 0.07 kg after 10 minute drying in the I. period. Calculate: a) period of time needed to reach the moisture content of $W_A = 0.07$, b) the moisture content after 70 min. of drying. Assume linear dependence of the drying rate on the moisture content of the material for the II. period of drying.

Solution: a)

The initial moisture content of the material is $W_{A0} = m_{A0}/m_C = 0.67/2.5 = 0.268$ and the critical one is $W_{Ac} = 0.14$. The drying rate of the I. period of drying is $N_{Ac} = (\Delta m_A/m_C)/\tau = (0.07/2.5)/10 = 2.8 \times 10^{-3} \text{ min}^{-1}$.

The period of time for the first period of drying will be calculated according to the equation:

$$\tau_1 = \frac{W_{A0} - W_{Ac}}{N_{Ac}} = \frac{0.268 - 0.14}{2.8 \times 10^{-3}} = 45.7 \text{ min}$$

The period of time in the second period for drying from $W_{Ac} = 0.14$ to $W_{At} = 0.07$ will be calculated from:

$$\tau_{II} = \frac{W_{Ac} - W_A^*}{N_{Ac}} \ln \frac{W_{Ac} - W_A^*}{W_{At} - W_A^*} = \frac{0.14 - 0.05}{2.8 \times 10^{-3}} \ln \frac{0.14 - 0.05}{0.07 - 0.05} = 53.7 \text{ min}$$

The total period of time of drying is $\tau_1 + \tau_{II} = 45.7 + 53.7 = 99.4 \text{ min}$.

b)

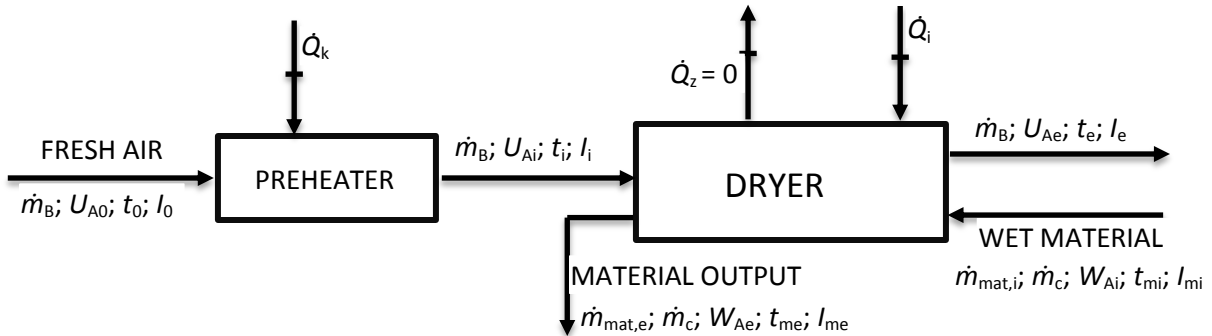
The period of time of drying in the first period is the same as in case a). In the second period the time of drying is $\tau_{II} = 70 - 45.7 = 24.3 \text{ min}$. On substituting into the equation for the second period of drying we get:

$$24.3 = \frac{0.14 - 0.05}{2.8 \times 10^{-3}} \ln \frac{0.14 - 0.05}{W_{At} - 0.05} = 53.7 \text{ min}$$

By solving this equation for W_{At} we obtain the final moisture content 0.092.

Enthalpy balance of the continuous dryer

5000 kg/hour of a wet material enters a continuous dryer. The material contains 45 wt. % of water. 3000 kg/hour of the material leaves the dryer. The highest allowed temperature of the material is 30°C and the critical moisture content of water is 5 wt. %. Air with temperature of 15°C and temperature of the dew point of 8°C is heated in a preheater. The relative humidity of air at the dryer outlet is 80%. Determine the consumption of air and the required heat input into the preheater. Assume no heat loss in the preheater and the dryer.



DATA: $\dot{m}_{\text{mat},i} = 5000$ kg/hour; $\dot{m}_{\text{mat},e} = 3000$ kg/hour; $w_{\text{Ai}} = 0.45$; $w_{\text{Ac}} = 0.05$; $t_0 = 15^\circ\text{C}$; $t_{\text{DP},0} = 8^\circ\text{C}$; $\phi_{\text{Ae}} = 80\%$; $t_{\text{max}} = 30^\circ\text{C}$;

We are to calculate: $\dot{m}_{\text{air},0} = ?$; \dot{Q}_k

SOLUTION:

Mass flow rate of dry material \dot{m}_c is:

$$\dot{m}_c = (1 - w_{\text{Ai}})\dot{m}_{\text{mat},i} = (1 - 0.45) \cdot 5000 = 2750 \text{ kg/hour}$$

The moisture content of the input and output material and the critical moisture content are:

$$W_{\text{Ai}} = \frac{w_{\text{Ai}}}{1 - w_{\text{Ai}}} = \frac{0.45}{1 - 0.45} = 0.8182$$

$$W_{\text{Ae}} = \frac{\dot{m}_{\text{mat},e} - \dot{m}_c}{\dot{m}_c} = \frac{3000 - 2750}{2750} = 0.0909$$

$$W_{\text{Ac}} = \frac{w_{\text{Ac}}}{1 - w_{\text{Ac}}} = \frac{0.05}{1 - 0.05} = 0.0526$$

The moisture content of the material leaving the dryer is larger than the critical one, $W_{\text{Ae}} > W_{\text{Ac}}$. Therefore, the temperature of the material is equal to the temperature of the wet-bulb thermometer and it must not exceed temperature of $t_w = t_{\text{max}} = 30^\circ\text{C}$. The temperature of the wet-bulb thermometer limits the temperature of air entering the dryer t_i . We will read off humidity, relative enthalpies and temperatures of the streams from the humidity chart:

1. fresh air: $t_0 = 15^\circ\text{C}$; $t_{\text{DP},0} = 8^\circ\text{C}$ ----> $U_{\text{A}0} = 0.00675$; $I_0 = 32.14 \text{ kJ/kg}_\text{B}$
2. air into the dryer: $U_{\text{A}i} = U_{\text{A}0} = 0.00675$; $t_w = 30^\circ\text{C}$ ----> $t_i = 80^\circ\text{C}$; $I_i = 101 \text{ kJ/kg}_\text{B}$
3. air from the dryer: $I_e = I_i = 101 \text{ kJ/kg}_\text{B}$; $\varphi_{\text{A}e} = 80\%$ -----> $U_{\text{A}e} = 0.0265$; $t_e = 33^\circ\text{C}$

The mass flow rate of the dry air will be calculated from the balance of the humidity/moisture content in the dryer:

$$\dot{m}_\text{B} U_{\text{A}i} - \dot{m}_\text{B} U_{\text{A}e} = \dot{m}_\text{C} W_{\text{A}e} - \dot{m}_\text{C} W_{\text{A}e}$$

$$\dot{m}_\text{B} = \frac{\dot{m}_\text{C} (W_{\text{A}e} - W_{\text{A}e})}{(U_{\text{A}i} - U_{\text{A}e})} = \frac{2750 \cdot (0.8182 - 0.0909)}{(0.0265 - 0.00675)} = 101.27 \frac{\text{t}}{\text{hour}}$$

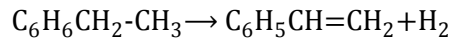
The overall amount of air will be $\dot{m}_{\text{air},0} = \frac{\dot{m}_\text{B}}{(1-U_{\text{A}0})} = \frac{101.27}{(1-0.00675)} = 101.96 \text{ t/hour}$. The heat input into the preheater will be calculated from the enthalpy balance of the preheater:

$$\dot{Q}_\text{k} = \dot{m}_\text{B} (I_i - I_0) = 101.27 \cdot 10^3 \cdot (101 \cdot 10^3 - 32 \cdot 10^3) = 6.988 \text{ GJ/hour.}$$

REACTORS

Tubular reactor (Dehydrogenation of ethylbenzene)

Dehydrogenation of ethylbenzene to styrene and hydrogen is carried out in a tubular reactor with inner diameter of 10 cm and length of 50 m filled with particles of catalyst. The reaction proceeds at 600 DC and 120 kPa. The reaction kinetics can be described by $r = kc_{EB}$, where r is the reaction rate. Reaction rate constant at 600 DC is $k = 0.0425 s^{-1}$. The molar flow rates of ethylbenzene and water vapor at the inlet of the reactor are $\dot{n}_{EB,0} = 0.025 \frac{mol}{s}$ and $\dot{n}_{H_2O,0} = 0.225 \frac{mol}{s}$. Calculate the conversion of ethylbenzene.



Solution:

1. Conversion will be calculated from: $X_{EB} = \frac{\dot{n}_{EB,0} - \dot{n}_{EB,e}}{\dot{n}_{EB,0}}$. The task is to determine the output molar flow rate of ethylbenzene.
2. The differential equation describing mass balance in a tubular reactor will be used.

$$\frac{d\dot{n}_{EB}}{dx} = -kc_{EB}A, \text{ where } A \text{ is the cross-section of the tubular reactor.}$$

3. We express c_{EB} as: $c_{EB} = \frac{\dot{n}_{EB}}{\dot{V}}$ and volumetric flow rate from the ideal gas state equation: $\dot{V} = \frac{\dot{n}RT}{p}$ where \dot{n} can be expressed as a function of \dot{n}_{EB} through the use of the extent of reaction:

$$\begin{aligned} \dot{n} &= \dot{n}_{EB} + \dot{n}_{H_2O} + \dot{n}_S + \dot{n}_{H_2} \\ \dot{n}_{EB} &= \dot{n}_{EB,0} + \nu_{EB}\xi \\ \dot{n}_{H_2O} &= \dot{n}_{H_2O,0} + \nu_{H_2O}\xi = \dot{n}_{H_2O,0} \\ \dot{n}_S &= \dot{n}_{S,0} + \nu_S\xi = \nu_S\xi \\ \dot{n}_{H_2} &= \dot{n}_{H_2,0} + \nu_{H_2}\xi = \nu_{H_2}\xi \end{aligned}$$

By combining all equations and substituting for stoichiometric coefficients we can arrive at: $\dot{n} = 2\dot{n}_{EB,0} + \dot{n}_{H_2O,0} - \dot{n}_{EB}$.

4. Substituting the derived expressions into the differential equation we get an equation that can be simply integrated: $\frac{d\dot{n}_{EB}}{dx} = -k \frac{\dot{n}_{EB}}{2\dot{n}_{EB,0} + \dot{n}_{H_2O,0} - \dot{n}_{EB}} A$

$$\begin{aligned} \frac{2\dot{n}_{EB,0} + \dot{n}_{H_2O,0} - \dot{n}_{EB}}{\dot{n}_{EB}} d\dot{n}_{EB} &= -kA \frac{p}{RT} dx \\ \int_{\dot{n}_{EB,0}}^{\dot{n}_{EB,e}} \frac{2\dot{n}_{EB,0} + \dot{n}_{H_2O,0}}{\dot{n}_{EB}} d\dot{n}_{EB} - \int_{\dot{n}_{EB,0}}^{\dot{n}_{EB,e}} d\dot{n}_{EB} &= -kA \frac{p}{RT} L \end{aligned}$$

$$(2\dot{n}_{EB,0} + \dot{n}_{H_2O,0}) \ln \frac{\dot{n}_{EB,e}}{\dot{n}_{EB,0}} - \dot{n}_{EB,e} + \dot{n}_{EB,0} = -kA \frac{p}{RT} L$$

$$(2 \cdot 0.025 + 0.225) \ln \frac{\dot{n}_{EB,e}}{0.025} - \dot{n}_{EB,e} + 0.025 = -0.0425 \cdot 0.0079 \frac{120000}{8.314 \cdot 873.15} 50$$

$$\dot{n}_{EB,e} = 0.0086 \text{ mol/s}$$

5. The molar flow rate at the reactor outlet is substituted into the relation for conversion:

$$X_{EB} = \frac{\dot{n}_{EB,0} - \dot{n}_{EB,e}}{\dot{n}_{EB,0}} = \frac{0.025 - 0.0086}{0.025} = 0.656$$

Results: The conversion of the ethylbenzene is 65.6 %.

Calculation of conversion in a cascade of CSTRs under isothermal conditions

Autocatalytic reaction $A=B$ is carried out in a cascade of 4 CSTRs with volumes of 0.5, 0.8, 1.5, and 2 m³, respectively. The input concentrations of the components A and B are 30 and 40 kmol/m³, respectively. The reaction rate constant is $1.7 \times 10^{-4} \text{ m}^3 \text{ kmol}^{-1} \text{ s}^{-1}$ and the reaction rate is described by $r = k c_A c_B$. The volumetric flow rate is 0.02 m³/s. Determine the output conversion of the component A.

A. Numeric solution:

The mass balance of component A for a kth CSTR reads:

$$(c_{A,k})^2 + \left(-c_{A,k-1} - c_{B,k-1} + \frac{\dot{V}}{v_A k V_k} \right) c_{A,k} - \frac{\dot{V}}{v_A k V_k} c_{A,k-1} = 0, \quad \text{where}$$

$$r_k = k c_{A,k} (c_{B,k-1} - c_{A,k} + c_{A,k-1}) \text{ was substituted for the reaction rate}$$

The mass balance for the 1. reactor:

$$(c_{A,1})^2 + \left(-c_{A,0} - c_{B,0} + \frac{\dot{V}}{v_A k V_1} \right) c_{A,1} - \frac{\dot{V}}{v_A k V_1} c_{A,0} = 0$$

$$(c_{A,1})^2 + \left(-30 - 40 + \frac{0.02}{-1 \cdot 1.7 \times 10^{-4} \cdot 0.5} \right) c_{A,1} - \frac{0.02}{-1 \cdot 1.7 \times 10^{-4} \cdot 0.5} 30 = 0$$

By solving this quadratic equation we obtain two solutions 25.2 and 280 kmol/m³. The requirement of $c_{A,1}$ be smaller than $c_{A,0}$ so that the system is physically meaningful, chooses the solution $c_{A,1} = 25.2 \text{ kmol/m}^3$. The corresponding concentration $c_{B,1}$ can be calculated from:

$$c_{B,1} = c_{B,0} - (c_{A,1} - c_{A,0}) = 40 + 4.8 = 44.8 \text{ kmol/m}^3$$

By repeating the same calculation from above for the other three reactors (substituting the corresponding values) we obtain the output concentration of the component A from the 4. reactor, that will be used for evaluating the conversion: $c_{A,2} = 18.7 \text{ kmol/m}^3$; $c_{A,3} = 10.6 \text{ kmol/m}^3$; $c_{A,4} = 5.05 \text{ kmol/m}^3$.

$$\text{Calculation of the conversion: } X_A = \frac{c_{A,0} - c_{A,4}}{c_{A,0}} = \frac{30 - 5.05}{30} = 0.83$$

B. Graphical solution:

1. We will rearrange the mass balance, so that it reads:

$$r_k = \frac{\dot{V}}{V_k} (c_{A,k} - c_{A,k-1}) \frac{1}{\nu_A} = -\frac{\dot{V}}{V_k} (c_{A,k} - c_{A,k-1})$$

At the same time the reaction rate is equal to: $r = k c_A c_B = k c_A (c_{A0} + c_{B0} - c_A)$, and this reaction rate can be plotted as a function of c_a in an interval of 0 to 35 kmol/m³ (blue line in graph below). We will use this graph to plot in the line given by the equation $r_k=f(c_{A,k})$ written for each of the four reactors (red lines). To plot a line we need two points or a point and a slope. The slope is given by the ratio of $\frac{\dot{V}}{V_k}$ and one point is $[c_{A,k-1}, 0]$. For the first reactor the slope is $-0.02/0.5=-0.04$ and the point has coordinates $[30,0]$. The intersection of the curves described by $r=f(c_A)$ and $r_1=f(c_{A,1})$ gives the output concentration $c_{A,1}$. By repeating the same process for the other three reactors, we obtain concentration $c_{A,4}$ that will be used for calculating the output conversion.

